Instituto Alberto Luiz Coimbra de
Pós-Graduação e Pesquisa de Engenharia

A METHODOLOGICAL APPROACH FOR INCORPORATING MATERIAL FLOW ANALYSIS INTO INTEGRATED ASSESSMENT MODELS: INTEGRATION BETWEEN THE COMPUTABLE FRAMEWORK FOR ENERGY AND THE ENVIRONMENT (COFFEE) AND THE OPEN DYNAMIC MATERIAL SYSTEMS MODEL (ODYM)

Leandro Costa Ferreira Gomes

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"Os homens fazem sua própria
história, mas não a fazem como
querem; não a fazem sob
circunstâncias de sua escolha, e
sim sob aquelas com que se
defrontam diretamente, legadas e
transmitidas pelo passado"
Karl Marx

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Resumo da Dissertação apresentada à COPPE/UFRJ como parte dos requisitos necessários para a obtenção do grau de Mestre em Ciências (M.Sc.)

UMA ABORDAGEM METODOLÓGICA PARA INCORPORAR A ANÁLISE DE FLUXO DE MATERIAIS EM MODELOS DE AVALIAÇÃO INTEGRADOS: INTEGRAÇÃO ENTRE O COMPUTABLE FRAMEWORK FOR ENERGY AND THE ENVIRONMENT (COFFEE) E O OPEN DYNAMIC MATERIAL SYSTEMS MODEL (ODYM)

Leandro Costa Ferreira Gomes

Fevereiro/2025

Orientadores: Alexandre Salem Szklo
Pedro Rua Rodriguez Rochedo

Programa: Planejamento Energético

Este estudo propõe uma abordagem metodológica para integrar a análise de fluxo de materiais aos Modelos de Avaliação Integrada (IAMs), abordando uma lacuna existente na modelagem climática e energética. Especificamente, explora a conexão entre o *Computable Framework for Energy and the Environment (COFFEE)*, um IAM desenvolvido na COPPE/UFRJ, e o *Open Dynamic Material Systems Model (ODYM)* em sua estrutura de *Resource Efficiency – Climate Change (RECC)*. Dado o papel crítico dos materiais na descarbonização, essa integração visa aprimorar a representação das restrições materiais nos cenários de transição energética.

A pesquisa inclui um diagnóstico detalhado dos modelos, avaliando suas estruturas, entradas, saídas e resoluções temporal e regional. Em seguida, identifica possíveis trocas de dados entre ambos, delineando os ajustes necessários na parametrização e na representação tecnológica para garantir compatibilidade. Uma contribuição central é a proposta de um fluxo de trabalho estruturado para a harmonização dos modelos, considerando as demandas setoriais por materiais, a dinâmica dos estoques e os ciclos de retroalimentação com os sistemas econômico e energético.

Este trabalho estabelece as bases para desenvolvimentos futuros, fornecendo um arcabouço para a vinculação da análise de fluxo de materiais aos caminhos de descarbonização abordados nos IAMs, permitindo a investigação da importância dos ciclos de materiais, das estratégias de eficiência de materiais e das possíveis limitações de recursos para o cumprimento das metas climáticas.

Abstract of Dissertation presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Master of Science (M.Sc.)

A METHODOLOGICAL APPROACH FOR INCORPORATING MATERIAL FLOW ANALYSIS INTO INTEGRATED ASSESSMENT MODELS: INTEGRATION BETWEEN THE COMPUTABLE FRAMEWORK FOR ENERGY AND THE ENVIRONMENT (COFFEE) AND THE OPEN DYNAMIC MATERIAL SYSTEMS MODEL (ODYM)

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This study proposes a methodological approach to integrating material flow analysis into Integrated Assessment Models (IAMs), addressing a standing gap in climate and energy modeling. Specifically, it explores the linkage between the Computable Framework for Energy and the Environment (COFFEE), an IAM developed at COPPE/UFRJ, and the Open Dynamic Material Systems Model (ODYM) in its Resource Efficiency – Climate Change (RECC) framework. Given the critical role of materials in decarbonization, this integration aims to improve the representation of material constraints in energy transition scenarios.

The research includes an in-depth diagnosis of COFFEE and ODYM-RECC, assessing their structures, inputs, outputs, and temporal and regional resolutions. It then identifies potential data exchanges between both models, outlining necessary adjustments in parameterization and technological representations to ensure compatibility. A key contribution is the proposal of a structured workflow for harmonizing the two models, considering sectoral material demands, stock dynamics, and feedback loops with economic and energy systems.

This work lays the groundwork for future developments, providing a framework for linking material flow analysis with IAMs decarbonization pathways, enabling the investigation of the importance of material cycles, material efficiency strategies and potential resource limitations in achieving climate targets.

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COFFEE	Computable Framework For Energy and the Environment	4
COPPE	Instituto Alberto Luiz Coimbra de Pós-graduação e Pesquisa de Engenharia	4
CR	Catalytic Reforming	187
DAC	Direct Air Capture	16
dMFA	dynamic Mass Flow Analysis	32
DRI	Direct Reduced Iron	187
EAF	Electric Arc Furnace	187
EAF	Electric arc Furnace	24
EoL	End of Life	121
EROEI	Energy Returned on Energy Invested	2
ETB	Ethanol-to-Butadiene	187
FCC	Fluidized Catalytic Cracking	187
FCV	Fuel Cell Vehicles	54
GE	General Equilibrium	8
GHG	Greenhouse Gases	3
GWP100	Global Warming Potential for a 100-year horizon	29
HB	Haber Bosch synthesis	187
HDD	Heating Degree Days	103
HDRI	Hydrogen Direct Reduced Iron	187
HERMES	Historical Trends For Mobility Assessment	100
HEV	Hybrid Electric Vehicles	54
HHDT	Heavy Duty Truck	101
HHE	Household Expenditures	22
HTH	High Temperature Heating	23, 187

HVAC	Heating, Ventilation and Air Conditioning	104
HVAC	Heating, ventilation, and air conditioning	24
HVC	High Value Chemicals	23
IAM	Integrated Assessment Models	4
ICCT	International Council on Clean Technology	22
ICED	Internal Combustion Engine, diesel	54
ICEE	Internal Combustion Engine, ethanol	98
ICEG	Internal Combustion Engine, gasoline	54
IE	Industrial Ecology	4
IMAGE	Integrated Model to Assess the Global Environment	38
IPCC	Intergovernmental Panel on Climate Change	4
IPPU	Industrial Processes and Product Use	7
LCA	Life Cycle Assessment	60
LCOE	Levelized Cost of Energy	20
LHDT	Light Duty Truck	101
LTI	linear time-invariant system	35
ME	Material Efficiency	60
MFA	Mass Flow Analysis	4
MFH	Multi-Family House	54
MHDT	Middle Duty Truck	101
MMV	Mixed Mode Ventilation	104
MSW	Municipal solid waste	24
MTA	Methanol-to-Aromatics	187
MTO	Methanol-to-Olefins	187
MTT	Metathesis	187

1 Introduction

The process of decarbonization to mitigate anthropogenic greenhouse effect entails a transition to energy sources with lower energy returns than current fossil-based sources (TRAINER, 2018), (MORIARTY and HONNERY, 2012), (MORIARTY and HONNERY, 2020), (HALL *et al.*, 2009), (MURPHY and HALL, 2010), which have been the foundation for industrial, population, and technological expansion over the last century and a half. The main alternatives emerging are wind and solar photovoltaic (PV) energy (SOLAUN and CERDÁ, 2019), (IRENA, 2016). Both face the issue of intermittency, requiring supplementary structures to mitigate this phenomenon (AGHAHOSSEINI *et al.*, 2017).

Beyond the primary sources themselves, transitioning to them involves a change in energy vectors and associated infrastructure. Essentially, greater electrification of the global energy matrix will be necessary. Combustion engine vehicles are likely to be replaced by electric motors, industrial processes will need to be electrified, and homes will need to be adapted, among other changes (DEETMAN *et al.*, 2021), (DEETMAN *et al.*, 2018). In other words, an entirely new productive structure will need to be facilitated, including the expansion of electric transmission (DEETMAN *et al.*, 2018), building adaptations (MARINOVA *et al.*, 2020), and the replacement of capital goods currently designed to operate and produce based on the paradigm of fossil fuel sources (DEETMAN *et al.*, 2021).

Additionally, in various decarbonization scenarios, a decrease in energy intensity is seen as a potential contribution to reducing greenhouse gases (CULLEN *et al.*, 2011), (GRÜBLER and NAKIĆENOVIĆ, 1996), meaning less energy will be required for the same activities. Again, there will be pressure for material changes in buildings, industries, infrastructure, and consumer goods to adapt to an energetically more efficient reality.

Given the scale of the transformations - whose time frame is proportional to the boldness of the mitigation goals - parts of the scientific community question the feasibility of these scenarios. Different approaches to this question vary; CULLEN *et al.* (2011), for example, attempts to quantify in detail how much energy demand can be reduced through efficiency alone. Regarding energy intensity, SEMIENIUK *et al.* (2021) discusses the feasibility of cutting demand, especially in poor and peripheral countries, where current demand is considered low by standards of a dignified life. Other approaches assess the feasibility of the transition from the perspective of the Energy Returned on Energy Invested (EROEI) ratio, which measures the energy surplus of an energy source, as seen in (TRAINER, 2018), (SGOURIDIS *et al.*, 2016), (HALL *et al.*, 2009), (HALL *et al.*, 2014), (LLOYD and FOREST, 2010), some even claiming the impossibility of maintaining our current sociometabolism as we know it (LLOYD and SUBBARAO, 2009) and (TRAINER, 2012). From the energy perspective, some authors - more or less optimistic - investigate the actual availability of these renewable energy resources (JACOBSON and DELUCCHI, 2011), (DE CASTRO *et al.*, 2011), (DE CASTRO *et al.*, 2013), and (CAPELLÁN-PÉREZ *et al.*, 2017).

Beyond the energy approach per se, a view of material feasibility is gaining traction (LO PIANO *et al.*, 2019), especially among groups working with integrated models (PAULIUK *et al.*, 2017), (BAARS *et al.*, 2022). Part of this approach also takes an energy perspective when it comes to mineral resource exploitation given that they undergo depletion, and, if technological advancement cannot outpace scarcity, exploitation becomes energetically costlier (RÖTZER and SCHMIDT, 2018), (NORTHEY *et al.*, 2014), (RÖTZER and SCHMIDT, 2020), (KOPPELAAR and KOPPELAAR, 2016). Along these lines, an analysis of the feasibility and viability of supplying certain critical materials is also necessary (GRAEDEL *et al.*, 2015),(SONG *et al.*, 2019),(ZENG *et al.*, 2022). It is known that copper will be more demanded in an electrification scenario; permanent magnet wind generators may strain the supply of neodymium; synthesis processes for biofuels require catalysts like cobalt; vehicle fleet electrification will strongly demand lithium, cobalt, nickel and other elements for batteries; crystalline silicon solar panels rely on silver for their contacts. There are concerns about whether sufficient reserves exist and or whether the rhythm of material supply (and investment) will meet the demand requirements. A peak in specific demand might not be met, potentially delaying the transition.Additionally, the current chokepoints may continue to be future constraints in maritime trade, and cuts in supply due to geopolitical issues could occur (OVERLAND, 2019). Still, in this regard, just as in oil production, where production is not always located at the point of consumption, some argue that transmission lines may become new ”chokepoints” or the new pipelines (OVERLAND, 2019).

Addressing these concerns, some authors and State institutions have attempted to tackle the problem more globally (MOREAU *et al.*, 2019), (U.S.DOE, 2011), (CARRARA *et al.*, 2020), (CHURCH and CRAWFORD, 2018) or specifically focusing on particular metals (LI and ADACHI, 2019), (LO PIANO *et al.*, 2019), (BONNET *et al.*, 2019), (ZENG *et al.*, 2022).

The focus on material analysis raises other motivating questions beyond feasibility. There are studies investigating the potential for Green House Gases (GHG) emission reductions via material efficiency (PAULIUK *et al.*, 2021d), (RISSMAN *et al.*, 2020), (FISHMAN *et al.*, 2021b), (PAULIUK *et al.*, 2021a); others that examine potential conflicts with the expansion of demand for certain materials in transition scenarios (EVANS, 2010); others that analyze social and environmental impacts, such as water use and land conflicts, in decarbonization scenarios (EVANS, 2010), (MUDD, 2008; NORTHEY *et al.*, 2016),(CAPELLÁN-PÉREZ *et al.*, 2017); others studying economic consequences in specific sectors due to high demand for certain materials (LO PIANO *et al.*, 2019) and, finally, some that debate potential geopolitical consequences of shifting demand from a fossil-based society to one based on renewable energy (CHURCH and CRAWFORD, 2018; HACHE, 2016; O'SULLIVAN *et al.*, 2017; OVERLAND, 2019; SQUIRE and DODDS, 2020; VAKULCHUK *et al.*, 2020).

Regardless of the approach, it is a fact that the exploitation and production of materials are responsible for a significant portion of GHG emissions and environmental impacts from human activity. Emissions from this sector can account for around 20% of the total depending on the year (HERTWICH *et al.*, 2019b), (PAULIUK *et al.*, 2021d), while it is estimated that the extraction of minerals, fossil fuels, and biomass combined are responsible for about 90% of biodiversity loss and water stress (UNEP-IRP, 2019). Therefore, strategies to mitigate emissions and environmental impacts of human activities must necessarily address this issue, both from the aspect of mitigation strategies through material efficiency and possible material constraints in mitigation scenarios. However, overall, there is a general consensus on the lack of linkage of economic mechanisms in material models and a shortage of mechanisms for material assessment in economic and/or energy models, as cited by BAARS *et al.* (2022). Thus, decarbonization scenarios envisioned within the framework of the Intergovernmental Panel on Climate Change (IPCC) Working Group III, developed using IAMs (Integrated Assessment Models), have a weak linkage with the transformations in material demand these scenarios will create (BAARS *et al.*, 2022) and (PAULIUK *et al.*, 2017). Additionally, the economic scenarios to which these IAMs are linked, usually provided by their respective CGE (Computable General Equilibrium) models, also fail to absorb impacts of price changes, rebound effects, and other potential outcomes from the transformation of the material sector's demand. From the perspective of material models, technological changes, choices, and price variations are not reflected in their demands over time (BAARS *et al.*, 2022). In this regard, there are initiatives from IAM groups and Industrial Ecology (IE) groups to integrate efforts to cover some of these gaps (PAULIUK *et al.*, 2021d), (PAULIUK *et al.*, 2021a), (FISHMAN *et al.*, 2021b), (PEDNEAULT *et al.*, 2022), (KLOSE and PAULIUK, 2023), (ZHONG *et al.*, 2021), and the current work fits into this approach.

1.1 Objective

In this thesis, a methodological proposal for integration between the IAM developed by the Energy Planning Program of COPPE, the COFFEE (Computable Framework For Energy and the Environment), together with its general equilibrium model, the TEA (Total Economy Assessment), and the Dynamic Material Flow Analysis model from the Industrial Ecology group at the University of Freiburg, the ODYM (Open Dynamic Material Systems Model) in its RECC (Resource Efficiency – Climate Change mitigation framework) version, is conducted.

1.2 Structure

In chapter 2, a literature review of the issues addressed in the thesis will be conducted. This chapter will briefly explain the differences between process-based and benefit-cost IAMs, with a greater emphasis on the later category, which includes the COFFEE model. Criticisms of IAMs, responses over time from their community, and possible new approaches will be raised. This will be followed by a more in-depth review of the potential of integrating IAMs with IE methods, focusing on the benefits of integration with the MFA (Mass Flow Analysis) method. Further, the MFA method will be explained in more detail, including the concept of convolution, the input-based and stock-based methods, the basic inputs, and values that are endogenous or exogenous to the model. Finally, the two models used in this work, the COFFEE IAM developed in the Cenergia laboratory of COPPE and the ODYM-RECC dynamic mass flow analysis model developed by the IE group of the University of Freiburg, are briefly addressed.

In chapter 3, the methodology used in the study is described. This chapter discusses how to systematically analyze the COFFEE model to identify its gaps, inputs, outputs, regional divisions, temporal resolution, loops, and detailed descriptions of technologies and processes, among others. The same process will then be applied to the ODYM model. Finally, the chapter discusses how to identify potential benefits of integrating both models and how to present the results.

In chapter 4, the results will be presented, including which outputs from COFFEE can be used as inputs for ODYM and vice versa. How constants, technologies, regions, and temporal resolutions should and can be adjusted will also be covered. There is an intention to present a decoding of the ODYM code that indicates parts of the code that should be changed in an implementation of the integration.

Finally, the conclusions are presented in the final chapter.

2 Bibliographic Review

2.1 Introduction to IAM

Integrated Assessment Models (IAMs) are pivotal tools in addressing climate change (CC), designed to evaluate mitigation strategies by integrating various aspects of human activities and environmental interactions (VAN BEEK *et al.*, 2020), (ROCHEDO, 2016, p. 37),(HAMILTON *et al.*, 2015). They provide insights into potential future scenarios under varying assumptions of economic growth, technological advancement, policy implementation, among others, serving as important tools for policymakers (KULKARNI *et al.*, 2024a).

IAMs encapsulate the complex interplay between technological, economic, and environmental systems. They are utilized extensively by the Intergovernmental Panel on Climate Change (IPCC), particularly by Working Group III (WGIII) (VAN BEEK *et al.*, 2020), (GAMBHIR *et al.*, 2019), to simulate the impacts and interventions related to climate change mitigation. These models operate by projecting future scenarios based on a range of inputs such as demographic trends, technological development, economic growth, policy changes and carbon budgets. The scenarios help in understanding the potential outcomes of different policy paths.

2.1.1 Types of IAMs

IAMs can be broadly categorized into two types: Benefit-Cost IAMs (BC) and Process-Based IAMs (PB) (GAMBHIR *et al.*, 2019) (KULKARNI *et al.*, 2024a) (also called Detailed Process (DP) IAMs (WEYANT, 2017)). Although both models incorporate forecasts of greenhouse gas (GHG) emissions and the costs associated with various mitigation strategies, they differ significantly in their structure (WEYANT, 2017).

Benefit-Cost IAMs focus on assessing the economic trade-offs of climate policies. They calculate the costs of mitigation measures against the potential damages avoided by them (GAMBHIR *et al.*, 2019), (WEYANT, 2017). Examples include the DICE model (Dynamic Integrated model of Climate and the Economy) and the PAGE model (Policy Analysis of the Greenhouse Effect). Despite being developed mainly in the context of the WG III, they are now more used in the context of WGII(PAULIUK *et al.*, 2017) (GAMBHIR *et al.*, 2019).

Process-Based IAMs provide a more granular view of the energy system and industrial processes, detailing specific technologies and their interactions with the economy and the environment (KEPPO *et al.*, 2021), (WEYANT, 2017)). They do not solely focus on cost-benefit analysis but aim to simulate physical and technological constraints. They also "provide more information on the physical impacts and economic costs of climate change and the benefits of GHG emission mitigation"(WEYANT, 2017).

The two types of IAMs differ significantly in their approach. Regarding their structure, Benefit-cost IAMs often use a top-down approach, starting with macroeconomic variables to assess overall economic impacts. Process-based IAMs frequently (but not exclusively) employ a bottom-up approach, focusing on specific sectors or technologies to build up a comprehensive picture (KOTCHEN *et al.*, 2023a). Regarding the level of details, process-based IAMs typically incorporate a higher level of detail regarding technologies, energy sources, and sector-specific dynamics compared to benefit-cost IAMs, which focus more on aggregate economic indicators (WEYANT, 2017), (GAMBHIR *et al.*, 2019), (HARFOOT *et al.*, 2014). In this thesis, we will focus on process based IAMs, a group to which COFFEE belongs.

2.1.2 Main characteristics of Process-based IAMs

Process-Based IAMs are mainly constitute by three modules or blocks (GAMBHIR *et al.*, 2019):

- An energy Demand Module: This component analyzes the demand for energy across various sectors, including industrial, residential, and transport, based on factors like economic activity, technological progress, and energy prices.
- Energy Supply Module: it assesses the availability and development of different energy technologies and their capacities to meet projected demand. It includes renewable energy sources, fossil fuels, and nuclear energy, considering factors such as resource availability, technological maturity, and policy constraints.
- A climate module: it measures the emissions from the energy system (an eventual additional blocks, like the land use and industry ones) in each timeframe and forecasts the resulting temperature changes throughout the model's projection period.

Many Integrated Assessment Models also capture the emissions from Industrial Processes and Product Use (IPPU) and other non-energy sectors, including land use, agriculture, industry, and waste management. These models account for both non-CO2 gases and CO2 emitted from sources other than energy. IAMs that do not explicitly consider non-energy system emissions can be integrated with individual sector-specific models or modules to address the emission of non-CO2 and CO2 gases.

Despite sharing a common framework, and beside differences in modules, process-based IAMs also differ in other several respects like:

Regional Representation: The regional division within IAMs aims to focus the analysis on specific geographic areas. Depending on the objectives and the country where the IAM was designed, the regional division varies considerably. For example, COFFEE, a Brazilian model, includes Brazil as one of its 18 regions. This separation allows for a better description of, for example, energy flows and agricultural products in the country. The table 2.1 compiles the regional division of some IAMs.

Temporal Resolution: Models vary in the granularity of their time steps, which can range from annual to multi-decade intervals, affecting the precision of their projections. Additionally, the final year can vary, but typically these models are run until the end of the century.

Sectoral Detail: The extent to which different economic sectors are detailed varies significantly, influencing the model's ability to pinpoint sector-specific mitigation strategies. Some examples of sectors covered by Integrated Assessment Models (IAMs) include energy, land use, industrial, residential, and transportation sectors.

Foresight Mechanism: Models may employ either perfect foresight or recursive-dynamic approaches. In the first approach, economic agents within the model are assumed to have complete knowledge of future states of the world throughout the model's time horizon. This means they can make optimal decisions today based on a full understanding of how those decisions will play out in the future. Models using perfect foresight can thus identify the most efficient paths to achieving long-term objectives, such as climate stabilization goals. This approach is commonly used in optimization models where the goal is to find the least-cost or most efficient strategy for the entire modeling period.

In the recursive-dynamic approach, models operate with a more limited scope of foresight. In this case, decisions are made one period at a time, based on current and past information only, without foreknowledge of future events or states of the world. This approach simulates a more realistic decision-making process, where agents adapt to new information as it becomes available over time. Each period's decisions depend on the outcomes of previous periods, making the model dynamically evolve. This method is particularly useful in simulation models.

Both foresight mechanisms have their merits and limitations: while perfect foresight provides clarity on optimal strategies, it may over-simplify real-world uncertainty and decision-making complexities. Recursive-dynamic models, on the other hand, offer a closer representation of how decisions are made in the real world but might not always identify the most efficient long-term strategies due to their segmented view of time.

Economic Agent Representation and Simulation vs. Optimization Models: In optimization models, economic agents are typically represented uniformly, often conceptualized as a single representative agent. This approach simplifies the complexity of human decision-making into a coherent, unified strategy that seeks to optimize a particular objective across the entire model. In those models, agents might be assumed to choose the same technology options based on what is most cost-effective or efficient for meeting the set goals, such as reducing emissions or minimizing costs. This method allows for a streamlined analysis of optimal paths but might overlook the diversity of behaviors and preferences that can occur in real-world settings (KEPPO *et al.*, 2021).

In contrast, simulation models allow for a more nuanced representation of economic agents. Simulations models provide the capability to represent a range of behaviors and decision-making processes across different agents or groups. This allows these models to account for variations in technology adoption, regional differences in policy implementation, and disparate economic priorities. As a result, simulation models can offer more detailed insights into how different policies might play out across various sectors and among diverse populations. This more granular approach in simulation models captures the complexity and heterogeneity of agent behaviors, which is crucial for understanding the potential impacts of policies in a more fragmented and decentralized economic landscape. Meanwhile, the uniform approach in optimization models, while less detailed in behavioral diversity, provides clear directives for policy by identifying the most efficient routes to achieve overarching goals. Both modeling approaches are instrumental in shaping informed and effective climate policies, each bringing a unique perspective to the strategic planning required to address global climate challenges.

Economic Coverage: Another distinction among IAMs relates to the scope of economic coverage, differentiating between Partial Equilibrium (PE) models and General Equilibrium (GE) models (or Computable General Equilibrium, CGE). PE models, such as many process-based IAMs, focus on specific sectors or markets, such as energy and agriculture, without accounting for the broader interactions with the rest of the economy (ROCHEDO, 2016, p. 90). These models assess the equilibrium in isolated markets, assuming that changes in these sectors do not significantly affect the overall economic landscape. This focus allows for detailed analysis within specific domains but does not capture the feedback effects that sector-specific changes might have on the entire economy.

In contrast, General Equilibrium models consider the interconnections and inter dependencies across all sectors of the economy. They assess how changes in one sector affect others, capturing the full economic feedback loops and allowing for a comprehensive analysis of economic policies and their impacts (GUNNING and KEYZER, 1995). GE models are particularly useful for examining the broader economic implications of environmental policies, such as carbon taxes, which might have widespread effects across various sectors (GUNNING and KEYZER, 1995).

Sometimes, the complexity of integrating all economic sectors into a single model leads to a hybrid approach, where a GE model operates linked with a PE model. In such cases, the PE model might provide detailed insights into specific sectors, while the GE model assesses the broader economic impacts, allowing for a more comprehensive analysis. CGEs can also provide IAMs with inputs from sectoral demand, such as energy (or energy services) and agricultural products demand (ROCHEDO, 2016, p. 90). This linkage between PE and GE models enables a more nuanced understanding of both sector-specific details and their macroeconomic consequences, providing a robust framework for evaluating the impacts of climate policies across an interconnected economic system. In table 2.1, reproduced in full from KEPPO *et al.* (2021), there is a summary of some major IAMs and their characteristics.

Table 2.1: General overview of some Integrated Assessment Models

Model	**Geographical Scope**	**Economic Coverage**[1]	**Solution Method**[2]	**Technology Detail**[3]	**Technological Change**	**Technological Diffusion**[4]	**Policy Instruments**[5]
REMIND-MagPIE	Global, 12 regions	REMIND: GE, MAgPIE: PE of the agricultural sector	REMIND: IO/NLP, MAgPIE: RD/S	High energy, high land-use	Partially endogenous for energy, endogenous agriculture productivity	High substitutability	Medium
MESSAGEix-GLOBIOM	Global, 11 regions	GE	IO/LP, GLOBIOM: RD/LP	High energy, high land-use	Exogenous energy conversion and energy end-use	High substitutability; Exp/Decl and SI constraints	Medium
IMAGE	Global, 26 regions	PE	RD/S	High energy, high land-use	Endogenous energy end-use, Exogenous material use and agriculture	Technology choice by mlogit functions; Exp/Decl and SI constraints	High
WITCH	Global, 17 regions	GE	IO/NLP	Low energy, low land-use	Endogenous (incl. R&D) energy and-use exogenous agriculture	Nested CES production function; Exp/Decl and SI constraints	Medium
ImaclimR-World	Global, 12 regions	GE	RD/S	Medium energy, no land-use	Endogenous energy conversion and end-use	Technology choices by logit functions; Exp/Decl and SI constraints	Low
TIAM-UCL	Global, 16 regions	PE	IO/LP	High energy, no land-use	Exogenous energy conversion and energy end-use	Exp/Decl constraints	Low
GEM-E3	Global, 46 regions	GE	RD/NLP	Medium energy, low land-use	Exogenous total factor, labour, Capital productivity, endogenous for low-carbon technologies	Mixed high/low substitutability; Exp/Decl constraints	Medium
E3M3-FTT	Global, 61 regions	Non-equilibrium demand-led	ME	High energy, low land-use	Endogenous energy conversion and energy end-use	Evolutionary modelling (replicator dynamics)	High
COFFEE-TEA	Global, 18 regions	COFFEE is PE, TEA is GE	COFFEE IO/LP, TEA is RD/S	High energy, medium land-use	Endogenous energy conversion, end-use, material use, Agriculture	Mixed high and low substitutability; SI constraints	High

[1] GE: general equilibrium (closed economy) and PE: partial equilibrium.

[2] IO/(N)LP: inter-temporal optimisation/(non) linear programming (perfect foresight); RD/S: recursive-dynamic/simulation; RD/(N)LP: recursive-dynamic/(Non) linear programming; ME: macroeconometric simulation

[3] Qualitative assessment based on (IAMC, 2020), with high/medium/low energy representation standing for detailed energy system/limited number of energy sectors/only electricity generation. For land-use high/medium/low represent the degree if coverage of land cover classes, agricultural commodities, and agriculture and forestry demands.

[4] Expansion and decline and system integration constraints.

[5] Based on (IAMC, 2020), with number of policies represented in the model (of max 14): Low ≤ 5, medium: 5–9, high ≥ 10.

Source (KEPPO *et al.*, 2021)

2.1.3 Gaps in IAMs and critics to them

Since they became the foundation of mitigation strategies by the IPCC in AR5, IAMs have undergone increased scrutiny by the scientific community (VAN BEEK *et al.*, 2020), (ROBERTSON, 2021). In this process, various authors have pointed out deficiencies, oversimplifications, lack of transparency, misguided premises, among other issues with these models. Some articles have compiled these criticisms and identified how the IAM community responds to such problems, as well as possible paths for still unresolved issues (ACKERMAN *et al.*, 2009), (GAMBHIR *et al.*, 2019), (KEPPO *et al.*, 2021), (PAULIUK *et al.*, 2017), (PETERS *et al.*, 2023). This section will address some of these critiques, providing specific examples and occasionally discussing how parts of the scientific community involved with IAMs have addressed them. This exposition will serve as a basis for pointing out which gaps dynamic MFA models might help to fill.

2.1.3.1 Lack of transparency on inputs and assumptions

According to KEPPO *et al.* (2021): "modeler judgment has an important role in defining numerous details about how the system is modeled (e.g. what technologies to include/exclude), but such subjective decisions, often driven by nonepistemic values and norms, are rarely made explicit", In that sense the transparency and clarity of IAMs in providing policy-relevant recommendations for long-term mitigation pathways have been under scrutiny. One major critique is the lack of transparency in key assumptions such as energy resource costs, technology constraints, and demand responses to carbon pricing. For example, Rosen's (ROSEN, 2015) highlights the unclear dependencies of IAM outputs on technology input assumptions. Despite IAM teams' efforts to address these criticisms by documenting models and input assumptions (IAMC, 2020),

Furthermore, there is ambiguity regarding what constitutes model outputs versus modeler inputs. Some studies assert the benefits of enhanced energy efficiency in achieving stringent mitigation goals, but it is often unclear whether these enhancements result from model algorithms or user-defined pathway storylines (ROGELJ *et al.*, 2015). This confusion arises because many IAMs emphasize detailed energy supply technologies over energy demand technologies, leading to uncertainties in model selections for scenarios like greater electrification or energy efficiency in transport.

Although, it is essential to clearly distinguish between model outputs and user inputs and to comprehensively document the assumptions and decision-making processes within these models, the approach that the IAM community has taken to address the problem is the adoption of common scenarios, such as the Shared Socioeconomic Pathways (SSP) (RIAHI *et al.*, 2017), which provide a framework for assessing how global changes in demographics, economics, technology, and environmental policies might influence climate mitigation and adaptation efforts. Another possible strategy to tackle the problem is to perform more in-depth sensitivity analysis to understand how key technology costs, performance parameters, and other inputs influence model results.

In addition to the Shared Socioeconomic Pathways (SSPs), there are several initiatives aimed at describing common pathways with an attempt to standardize some input and output data, such as the ENGAGE consortium, CD-Links (CD-LINKS, 2024), and the development of a platform for describing IAMs (IAMC, 2020). Nevertheless, there are criticisms (PETERS *et al.*, 2023) suggesting that Working Group III should align more closely with the methodology of common frameworks adopted by Working Group I through the Coupled Model Intercomparison Project (CMIP) (WORLD CLIMATE RESEARCH PROGRAMME, 2024).

2.1.3.2 Representation of Material Cycles

Part of the premise behind the construction of IAMs is the organization of sociometabolism to meet the well-being of humanity, which includes providing fundamental services like water and food, welfare services such as housing, interconnection services like communication and transportation, and cultural services such as art and education. These services are facilitated by the transformation of resources available in the surrounding environment within social structures. Sociometabolism, when internalizing resources from the external environment, transforms them into flows and stocks of materials. Part of these flows become energy flows. Both have their equivalence in terms of material and energy services provided. A simple schematic is presented in figure 2.1.

While IAMs specialize in modeling the energy flows of these services, they address material flows and stocks only marginally. Some IAMs represent the production of bulk materials, usually steel and cement, but it is generally driven by a relationship of demand linked to GDP growth or per capita GDP. There are no correlations, for example, between the demand for these materials and the amount of stock added from built area or transportation infrastructure added (PAULIUK *et al.*, 2017). In (PAULIUK *et al.*, 2017), it is demonstrated how GDP or per capita GDP are variables with low correlation to the consumption of some materials. The variable that better describes the increase in demand for certain materials is the stock, both what is available at the beginning of the analysis and its increase over a time interval. Thus, a 3% GDP growth in a country with already developed infrastructure, such as France, has a very different impact on the increase in steel demand compared to GDP growth in a developing country where this increase is more likely to occur

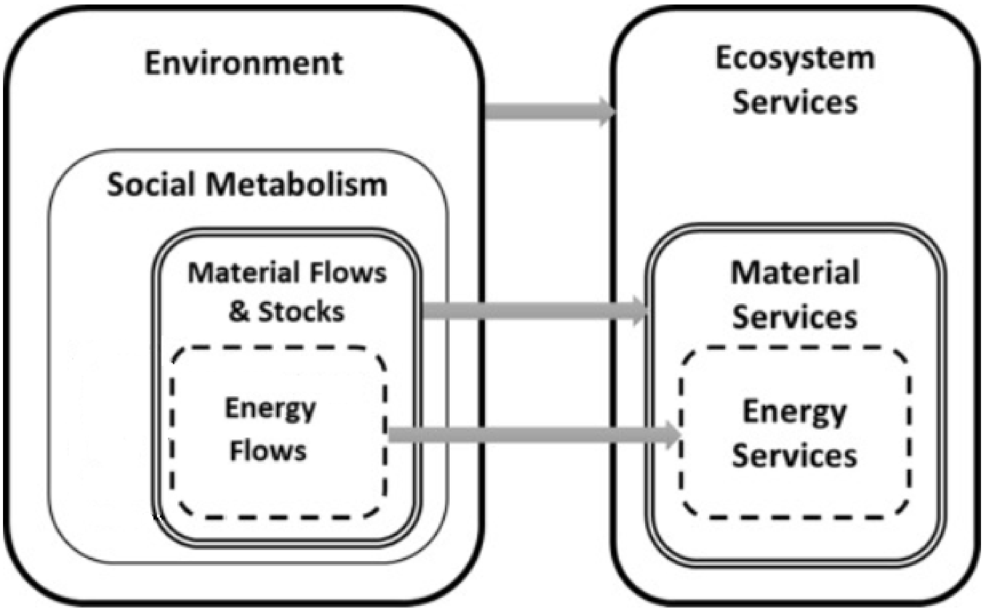


Figure 2.1: Link between material and energy flows and stocks and their respective services. (Source: (WHITING *et al.*, 2020))

in sectors demanding materials such as transport infrastructure and housing, for example.

Regarding the low representation of material cycles and its stages [1], activities such as production, manufacturing, stocks in use, waste management, and recycling are usually aggregated, and others, such as mining, are not even represented. This aggregation overlooks the potential to explore scenarios of material efficiency, mitigation through better material uses, increased recycling, and the use of products with lower material intensity (PAULIUK *et al.*, 2021d).

Due to their primary focus on the energy system, Integrated Assessment Models (IAMs) generally do not work with mass balances (an exception can be made for carbon emissions). As mentioned above, the assessment of materials is typically conducted using a correlation with macroeconomic indices, a top-down approach. Thus, the production of a material assessed in this way may not correspond to the demand that would be derived from a bottom-up analysis, which, broadly speaking, would aggregate the demand for that material for each consumer good produced. Another aspect is that data on the life distribution of assets and stocks are only available for energy-related items, and occasionally for transportation and residential applications (PAULIUK *et al.*, 2017). Moreover, this distribution is linear rather than based on a typical probabilistic distribution (such as Weibull or Gaussian). An asset is retired from use when a certain fixed age is reached.

[1] Section 2.3.2 will detail this discussion, e.g. see Figure 2.6

2.1.3.3 Issues in modeling technology diffusion and dynamics

Integrated Assessment Models (IAMs) have been criticized for their ability to accurately capture the diffusion of technologies and the factors influencing the dynamics and forms of these transitions. Critics argue that IAMs often overlook the evolution of technologies within their broader contexts, leading to challenges in capturing the drivers of path dependencies, market dynamics, and innovation. Some IAMs may present outcomes for key technologies that are either too optimistic (e.g., extensive use of BECCS [2]) or too pessimistic (e.g., low penetration of PV generation) (GAMBHIR *et al.*, 2019), indicating a need for improved modeling of endogenous technological change. Technological learning, which has historically shaped energy transitions by reducing costs and increasing efficiency, is represented variably across IAMs. Some models incorporate endogenous learning curves, typically showing a relationship between installed capacity and cost, while others rely on exogenous cost trajectories that are directly inputted (KEPPO *et al.*, 2021). However, in reality, technological learning depends on numerous factors that are difficult to model within IAMs.

The ability of IAMs to capture the real-world speed of technology deployment is also questioned. Models often impose exogenous constraints on the speed of technology diffusion rather than modeling these limits endogenously. Similar to technological learning, factors influencing deployment speed—such as energy policies, niche markets, technology characteristics, and public acceptance—are complex and numerous, making them challenging to fully represent in models. Historically, IAMs have used constraints like expansion and decline limits or multinomial logit functions to moderate investment growth and prevent unrealistic outcomes. Depending on the limitations imposed by the modeler, one might encounter the problems discussed earlier (KEPPO *et al.*, 2021). System-level characteristics, such as technology substitutability and system integration requirements, further affect the speed and extent of market share changes, with IAM outputs sometimes qualitatively matching historical diffusion dynamics but varying in optimism or conservatism.

To address these issues, recent IAM research has explored alternative modeling approaches that better represent technology adoption and diffusion. This includes incorporating complexity dynamics, agent heterogeneity, and heterogeneous consumer groups with varying preferences (MERCURE *et al.*, 2016). Additionally, integrating more empirical evidence into diffusion equations and frequently updating technology data can enhance model accuracy.

[2] Bioenergy with Carbon Capture and Storage

2.1.3.4 Out of date data and common date and data baselines

Integrated Assessment Models (IAMs) have been criticized for using outdated, inappropriate, or unknowable input assumptions. For example, the AR5's shown scenarios starting rapid mitigation from 2010, despite its 2014 release. Another example, some IAMs used cost projections from 2008, significantly overestimating current solar PV costs (GAMBHIR *et al.*, 2019). This highlights the necessity for IAMs to use updated data to accurately reflect the potential of emerging technologies in climate mitigation. Critics like Rosen and Guenther argue that due to substantial uncertainties and transformations in the energy system, long-term cost predictions for climate mitigation are inherently unknowable, suggesting a focus on short- and medium-term.

Additionally, there are variations in base year data across different IAMs. For example, Gahmbir et al. (GAMBHIR *et al.*, 2019) points a discrepancies in energy and emissions data for the base year, often around 2010. Krey at al. (KREY *et al.*, 2019) identifies expressive divergences in techno-economic characteristics in the electric sector between different IAMs. This inconsistent starting points may make future mitigation efforts seem easier or less costly than they truly are.

The dependence on baseline assumptions presents challenges for IAMs. The future economy and energy system can develop along numerous pathways, leading to a wide range of potential scenarios. So, addressing these variations is crucial, as differing base year energy demand values can significantly impact the perceived mitigation effort required to meet temperature goals. Improved alignment and transparency in data sources used by various modeling groups would enhance the robustness of IAM projections. In that sense, the introduction of shared socioeconomic pathways (SSPs) aims to address this by offering a range of baseline cases, from fossil fuel-intensive to low-carbon and energy-efficient scenarios.

2.1.3.5 The overlooked cost of inaction

IAMs are essential for comparing the costs and benefits of various climate policies and have been pivotal in advising policymakers on cost-effective greenhouse gas emission reduction pathways based on economic factors (KULKARNI *et al.*, 2024b). However, the economic costs of climate change, particularly those linked to extreme events such as Hurricane Harvey(ROBERTSON, 2021), may be evolving differently and at a faster rate than current IAM-based damage functions can accommodate (FRAME *et al.*, 2020), (KULKARNI *et al.*, 2024b). KOTCHEN *et al.* (2023b). Critics like STERN (2016) also argue that IAMs' baseline cases often overlook the potential economic disruptions caused by unchecked climate change or the costs associated with local air pollution from business-as-usual scenarios (HOWELLS *et al.*, 2013). This discrepancy emphasizes the necessity to enhance IAMs to better reflect the changing landscape of climate-related economic disruptions which could provide a more comprehensive understanding of the true costs and benefits of climate action (BUREAU *et al.*, 2021).

2.1.3.6 Feasibility

A common criticism of Integrated Assessment Models (IAMs) is the lack of feasibility checks for some of the adopted assumptions and obtained results. For example, in MAIA *et al.* and GAMBHIR *et al.* (2019), the feasibility of adopting Carbon Dioxide Removal (CDR) measures such as Direct Air Capture (DAC) and BECCS in more stringent scenarios is questioned. The concerns arise regarding the constraints these scenarios would impose in terms of material demand, energy, land use, water use, among others. While some studies indicate a significant role for BECCS in their scenarios, they also acknowledge that land use restrictions, biodiversity preservation, water management, and other factors could reduce biomass availability by 40 to 90% in Europe (BÉRES *et al.*, 2024).

Another controversial point is the assumption of decoupling energy demand, (and potentially, also material demand) from GDP growth (IEA, 2019), especially in scenarios with lower carbon budgets. This aspect also faces strong criticism, as in (NIETO *et al.*, 2020), which discusses the feasibility of this assumption. Historical data analysis shows that such decoupling rarely occurs in reality. STECKEL *et al.* (2013) and SEMIENIUK *et al.* (2021) examine how this decoupling, particularly for developing countries, means maintaining these populations in a scenario of energy poverty. Meanwhile, CULLEN *et al.* (2011) attempts to estimate the thermodynamic limits of efficiency gains, a crucial factor for decoupling.

A third line of approach concerns the demand for materials to meet the considered scenarios. A transition to renewable sources generally implies the electrification of systems previously fueled by fossil sources, such as boilers and internal combustion engines. ZENG *et al.* (2022) assess the supply of cobalt via dMFA methods and identify supply constraints in the near future. While LO PIANO *et al.* (2019) evaluates the silver constraints for contacts in silicon PV panels. HENCKENS (2022) assess the demand for certain minerals for the energy transition in a long-term view, stating that there could be supply limitations from the perspective of reserve availability.

Developing tools that can feed back into IAMs regarding the feasibility of scenarios and providing new constraints is crucial for enhancing the reliability of the results provided.

2.1.3.7 Representation of heterogeneity within and across actor groups

IAMs are typically constructed using concepts from orthodox classical economics, such as perfect markets and rational agents who seek to maximize their utility functions. Economic agents are usually represented as homogeneous (MERCURE *et al.*, 2016) and without information asymmetry (KÖHLER *et al.*, 2019), thus, all adopt the same allocative strategy depending on cost and constraints. For example, a particular cheaper generation technology is adopted until its constraints are met before the adoption of a expensive one. This modeling approach tends to simplify the complexity of the economic environment and does not adequately describe the heterogeneous behavior of various actors and their allocative choices.

KEPPO *et al.* (2021) mention a certain complexity in this area. Modeling heterogeneity essentially means modeling the specificities of various economic agents. While it is stated that the literature indicates heterogeneity is closely linked to societal transitions (necessary in a mitigation scenario), it is also asserted that specificity modeled over distant horizons tends to not bring accuracy in results.

Another problem pointed out in GAMBHIR *et al.* (2019) is that the models are based on a least-cost objective functions. Technologies that embed efficiency in cost tend to be cheaper and therefore are predominantly adopted in the models. However, there are cases, such as in developing countries, where the energy market functions poorly and there is a greater dependency on traditional fuels - making it impossible to adopt certain technologies like electric cars - or even a preference for more reliable traditional sources instead of dealing with the intermittency of PV and wind power.

2.1.3.8 Energy and economic feedbacks

Integrated Assessment Models (IAMs) have faced criticism for their representation of the economy. As exposed in the previous section, IAMs have been criticized for relying on idealized economic assumptions of perfectly functioning markets, which overlook significant real-world frictions that influence macroeconomic dynamics and cost assessments. Furthermore, IAMs have been critiqued for their approach to capturing energy-economy relationships and feedback mechanisms (KEPPO *et al.*, 2021). According to Hourcade et al. (HOURCADE *et al.*, 2006), IAMs based on 'conventional Top-Down' models often fail to adequately represent technological flexibility and the possibilities and limits of substitution. For instance, the use of constant elasticity of substitution (CES) functions for energy modeling has been shown to poorly match historical energy transition patterns (KAYA *et al.*, 2017).

Conversely, IAMs that follow a Bottom-Up approach without incorporating macroeconomic modules (CGE), fail to represent the macroeconomic feedbacks of different energy transition pathways. These pathways include rebound effects, investments, and household expenditure impacts on the economy (KEPPO *et al.*, 2021).

Some models do not account for the economic loop closure for new investments in productive infrastructure (such as industries and energy generation), meaning they do not subtract the investment budget from the total available consumption budget. By not doing this, they indirectly break a link with the biosphere. As a result, changes in the value of certain materials, or in the value of carbon, for example, do not lead to a new budget constraint, making the choice of certain energy sources or technological and industrial options more flexible (PAULIUK *et al.*, 2017). Models that do incorporate this closure typically do so via a soft-link with a Computable General Equilibrium (CGE) model. This integration allows for a more realistic simulation of economic dynamics, where investments impact available resources and enforce more stringent decision-making criteria based on environmental and economic feedback loops.

In the next section, we will specifically analyze the IAM COFFEE and its associated CGE model, which are intended to be integrated with ODYM-RECC.

2.2 COFFEE-TEA

2.2.1 COFFEE

The COFFEE IAM, developed in 2016 as part of a doctoral thesis at COPPE/UFRJ's Energy Planning Program, represents an advanced Integrated Assessment Model (IAM) (ROCHEDO, 2016). It integrates energy systems, land use, and socio-economic dynamics to evaluate the efficacy of climate policies globally, with a particular emphasis on Brazil, that represents one of its 18 regions, as seen in figure 2.2 and described in table 2.2. This model addresses the need for incorporating perspectives from developing countries in global climate change assessments, which are often underrepresented in existing IAM frameworks. It utilizes established modeling techniques and applies them to incorporate regional specifics, highlighting the environmental and economic conditions of Brazil and other non-OECD countries.

COFFEE IAM is grounded in the foundations of the MESSAGE model (Model for Energy Supply Strategy Alternatives and their General Environmental Impact), a partial equilibrium IAM from IIASA (International Institute for Applied Systems Analysis). The COFFEE was later coupled with a CGE model, the TEA, enabling assessment of economic impacts across diverse sectors. The integration of these models enables an analysis that links economic activities with energy supply and consumption, allowing for a thorough assessment of policy impacts on different future

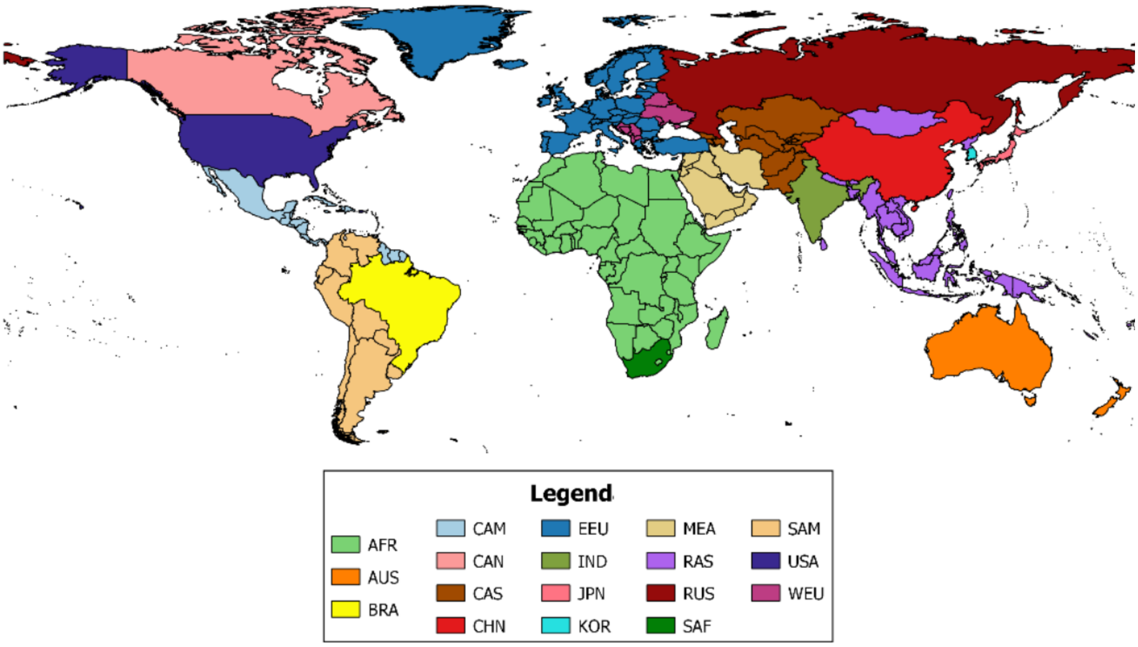


Figure 2.2: The 18 regions in COFFEE (Source: (ROCHEDO, 2016, p. 48))

scenarios.

Regarding the time horizon and resolution, COFFEE operates from 2010 to 2100 in 14 time intervals, with potential adjustments in this resolution to accommodate various modeling needs. As for the scope of greenhouse gases, it evaluates emissions of carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O). The economic component of COFFEE IAM covers the energy, transportation, industrial, residential, services, agriculture and residues sectors. Each sector is analyzed to understand its specific energy demands and economic implications.

2.2.1.1 Energy Sector

Figure 2.3 (source: (ROCHEDO, 2016, p. 51)) illustrates the energy structure of the model for each region. Energy systems convert resources into primary energy, which is then transformed into secondary and ultimately final energy. These energy levels can be exported to or imported from other regions based on constraints and costs. For example, regions with little or no oil resources, or with high production costs, may need to import energy. Once the necessary energy vectors are produced, exported, or imported, they are delivered to final consumer sectors. In each sector, final energy sources are converted into required energy services. Energy services are the end goal of energy use. For example, the transport sector demands the passenger kilometer (pkm) or tonne kilometer service for cargo transport, which can be supplied by different types of secondary energy. In the other hand the industrial sector utilizes various energy forms to produce heat, steam, driving force, lighting, cooling, and more. Each sector's energy services represent the exogenous demand

Table 2.2: Description of the 18 regions (Source: (ROCHEDO, 2016, p. 49))

Tag	**Description**
AFR	Africa (except South Africa)
AUS	Australia and New Zealand
BRA	Brazil
CAM	Central America
CAN	Canada
CAS	Caspian Region
CHN	China
EEU	East European (EU)
IND	India
JPN	Japan
KOR	South Korea
MEA	Middle East
RAS	Rest of Asia and Oceania
RUS	Russia
SAF	South Africa
SAM	South America (except Brazil)
USA	United States
WEU	West Europe

that the model aims to fulfill at the lowest cost. The energy sector is distinct from other ones analyzed in the model: while the others drive energy demand through economic development, the energy sector responds to the energy demands of the other economic sectors, either locally or from other regions.

The model deals with the estimation of reserves and resources of oil, natural gas, coal, uranium, and classifies them into slots (or steps) of production or extraction cost per available quantity. For renewable energies, it employs a similar approach, but uses the Levelized Cost of Energy (LCOE) for each production region instead of extraction costs. Each major type of renewable energy source is further divided into subtypes, such as small and large hydro potential for hydroelectric energy. Additionally, the model evaluates the potential of reservoirs for carbon capture and storage (CCS), treating these as a non-energetic resource. The energy sector involves resource extraction and transformation of these resources from primary to secondary and final energy forms, and is divided into three main categories (subsectors): Refining, Power, and other fuels.

The refining sector is partially modeled in a model external to COFFEE, called the Carbon and Energy Strategy Analysis for Refineries (CAESAR). In this software, the production profile and utility consumption of refineries are modeled. Additionally, six different types of crude oil and 18 process units are modeled. Thus, for example, a demand for diesel can be met by various combinations of unit use within each refinery, based on different crude oil typologies, which will also result in a different production profile of products. In this scheme, energy consumption and an emission factor are associated with each unit, allowing for the calculation of energy consumption and GHG emissions per produced product. It is worth noting that this level of detail is somewhat uncommon in most Integrated Assessment Models (IAMs).

For the electric sector, more than twenty energy sources and over 100 technologies are modeled, including those with Carbon Capture and Storage (CCS). This extensive modeling allows for a comprehensive analysis of the potential environmental impacts and energy efficiencies across a diverse range of technologies and energy sources in the electric sector.

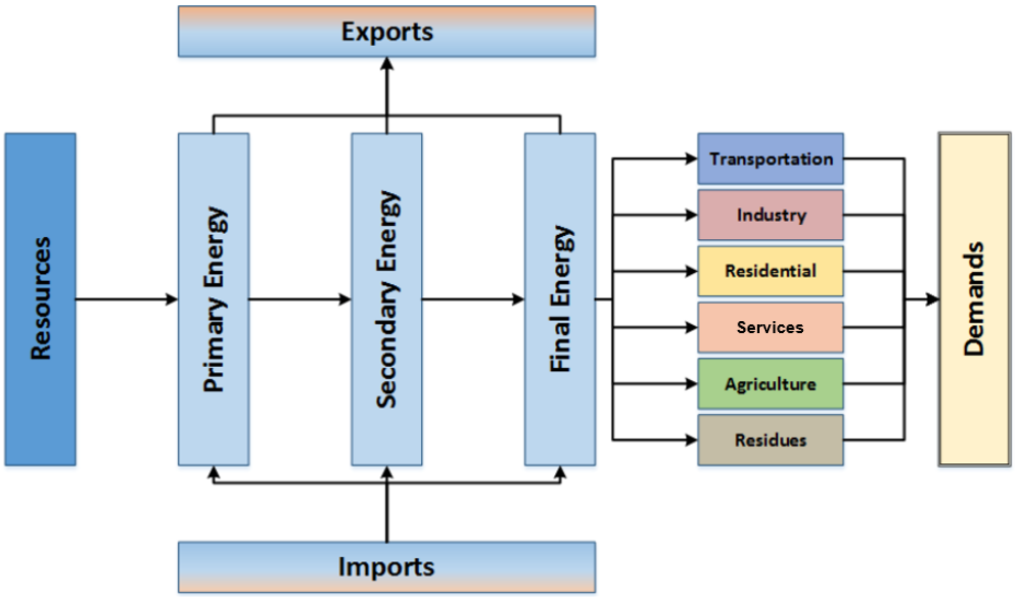


Figure 2.3: The energy transformation structure in COFFEE (Source: (ROCHEDO, 2016, p. 51))

2.2.1.2 Transportation Sector

The demand in the transportation sector is calculated exogenously to COFFEE or TEA using a model based on the one from the International Council on Clean Technology (ICCT, 2012), which includes the following modes: Light Duty Vehicles (LDVs, including SUVs), buses, 2-wheelers (2W), 3-wheelers (3W), Light Heavy Duty Trucks (LHDTs) (5,750 – 14,000 lbs), Medium HDTs (MHDTs) (14,000 – 33,000 lbs), Heavy HDTs (HHDTs) (>33,000 lbs), passenger rail, freight rail, aviation (passenger only), and marine for freight only. The original model, divided into 11 regions, had to be adapted to the 18 regions of COFFEE. From the technology perspective, it includes: internal combustion engines, hybrids, plug-in hybrids, fuel cells, and battery electric vehicles. Regarding fuels, it accounts for: diesel (conventional and low-sulphur), ethanol (grain, sugarcane, cellulosic), biodiesel (oil-based, ligno-cellulosic), natural gas, LPG, hydrogen, electricity, jet fuel, and fuel oil (ROCHEDO, 2016)

The ICCT model incorporates a large array of input data that has not been altered. This data includes region-specific average passenger occupancy (passengers per vehicle), typical mileage (km per year), historical fleet by region, and fleet composition by type and technology, among others. The economic input data of the model (such as GDP, population, and prices based on IEA scenarios) are then adapted to match those used in COFFEE, while maintaining the constants of the Gompertz demand elasticity curves used in the model which serve to calculate future service demand. In order to explore mitigation scenarios, options for shifting from less efficient to more efficient modes, as well as new technologies, have been added to the model.

2.2.1.3 Residential Sector

The residential sector's energy consumption is directly linked to the size of the population and factors such as income, consumption patterns, and social structure. In COFFEE, residential energy consumption is addressed using the number of households. Initially, an estimate from UNSTAT is used for the number of residents per dwelling in each region. This factor is projected over time in conjunction with the evolution of Household Expenditure (HHE). Consumption per household is categorized into six energy services: water heating, space heating, cooking, lighting, refrigeration, and appliances. Each region has a specific energy service intensity per dwelling, which can be met by various energy sources. Beyond merely using these factors, COFFEE employs more sophisticated methods to estimate the evolving demand for space heating and cooling services, utilizing regionalized Heating Degree-Days (HDD) and Cooling Degree Days (CDD). These methods allow for a more precise forecasting of energy requirements related to residential heating and cooling.

2.2.1.4 Service Sector

The services sector encompasses a diverse range of activities such as hospitals, banks, governmental institutions, schools, etc. In COFFEE, the approach to estimating energy consumption in this sector is similar to that used for the residential sector, but it utilizes floor space as the driver instead of the number of establishments. Given the sector's variety in function, space usage, and area demand, this approach was preferred. For estimating future built-up area, the model uses data on current built-up area and the GDP per capita of the service sector to derive an area intensity factor per GDP. By intersecting this with future GDP values for services (input into the model), the final floor area is obtained. Lastly, energy intensity factors per area are used for each of the same six energy services addressed in the residential sector.

2.2.1.5 Industrial Sector

The industrial sector in COFFEE recently underwent significant changes that provided greater detail. This section is based on the doctoral thesis of ZOTIN (2024), in which these modifications were developed.

The industrial sector comprises the following sectors: cement, iron and steel, chemicals, which includes High Value Chemical (HVCs), ammonia, methanol explicitly mdelled and other chemicals, and other industries. For this sector, the energy service demand is more important than the energy consumed. The model considers the following energy services: direct heating; steam (for indirect heating or for machinery operation); motive power (by electricity or fuels); lighting; heating, ventilation, and air conditioning (HVAC) of indoor areas; and finally, a category labeled "others" for residual services. The "others" category is essentially the difference between the demand described by the IEA and the demand from the cement, chemicals, and iron & steel sectors. These energy services can be primarily met by two energy vectors: fuels or electricity.

The demand of the industrial sector is given exogenously to the model, driven by macroeconomic variables such as GDP, GDP per capita and population. It may come from pre-established economic scenarios or from runs of the associated CGE, TEA. It is important to note that the model also accounts for non-energy demand, which refers to the consumption of products typically used as fuels but utilized as raw materials in industrial processes. Being supplied by the industrial sector, their demand must be counted to replicate demand in the energy sector. Some examples include natural gas used in fertilizer synthesis, naphtha in petrochemicals, and coal in steelmaking processes.

For the subsectors modeled within the industrial sector, the demand for each material can be met through different routes. Each route has an associated investment plus O&M cost, energy demand, and GHG emissions, which will be optimized within the run depending on the constraints set in each scenario. The steel subsector, for example, is modeled through 14 production technologies across three main routes: integrated, sponge iron, and electric arc furnace, some of which include carbon capture and storage (CCS) technologies. Cement production is divided into three stages— High Temperature Heating (HTH) generation, clinker production, and cement mixing—each with multiple pathways and energy options. Chemicals production is split into HVC, methanol, ammonia and a broader sector comprehending others chemicals.

Finally, for the industrial sector, in addition to emissions related to energy consumption, emissions intrinsically linked to industrial processes such as the production of cement, ammonia, and steel are accounted for.

2.2.1.6 Waste Sector

The waste sector differs from the others in that it does not involve the production of a final good. Moreover, its emissions are not from energy use but from the decomposition of waste, which primarily generates methane and nitrous oxide, or from incineration. Although it is not a major emissions sector, it has been considered for two reasons: first, the methane produced can serve as an alternative fuel, such as in waste-to-energy (W2E) options. Second, the two typical gases from emissions have a greater short-term impact on global warming than CO_2. Additionally, in the future, the model could be enhanced with changes in behavior concerning waste generation, collection, disposal, and composition.

As a source of generation, Municipal Solid Waste (MSW) was considered (effluents from the agriculture sector were included in the agriculture module described later). Based on World Bank data (WORLD BANK, 2012), the following waste disposal and/or destination types were considered for each region: dumpsites, landfills, composting, recycling, W2E, and incineration. Furthermore, the composition was also considered in the following elements: organic, paper, plastic, glass, metal, and others. Each combination of composition by type of destination results in an emission factor. Such emissions can be used in energy conversion processes with associated costs expressed in LCOE for each type of destination.

Finally, the evolution of demand is also exogenous and given by a correlation between Household Expenditure (HHE) and waste generation per kg/hab/day.

2.2.1.7 Agriculture and Land Use Sector

COFFEE also includes a module addressing land use, land-use change, agriculture, and livestock management. This is particularly relevant for Brazil, where land-use changes constitute the primary source of national emissions (OBSERVATÓRIO DO CLIMA, 2024). Furthermore, the agricultural sector plays a crucial role in the national GDP (CENTRO DE ESTUDOS AVANÇADOS EM ECONOMIA APLICADA (CEPEA), ESALQ-USP, 2024), contributing to both non-energy and energy products, such as ethanol and biodiesel. It's important to note that the significance of the biofuels sector is mirrored in other countries, considering that more than 50 countries currently have biofuel blending mandates (TRINDADE *et al.*, 2022).

In this IAM, land can exist in three states: forest (native vegetation), pasture, or plantation. Forests may be converted into pastures through deforestation and may also be reforested. Pasture land can be transformed into plantation land and vice versa. Plantation areas cater to specific crop demands, while pastures support the production of animal protein. Similarly to energy demand, the demand for land-derived products can be satisfied through regional production or imports, with a portion of the output potentially exported to other regions.

The land use module within the MESSAGE model utilizes a non-spatially explicit approach to optimize land use to meet the demand for food and bioenergy products. Land categories or zones were established where aspects such as vegetation cover, soil productivity, and cost estimates for production were assigned.

Seven types of land cover were considered: forests, forest-grassland, grasslands, crop-vegetation and cropland. Other two types are part of the coverage that includes water bodies and lands considered ”not suited”, which encompass urban areas, desert regions, or areas permanently covered with ice.

Production costs were determined by combining two factors: land productivity and the transportation cost of production. For productivity, soils were characterized using the ”Productivity Index (PI),” which is normalized and ranges from 0 to 100. Despite being a simplification, this index incorporates factors like pH, moisture, nutrients, among others, and serves both as a proxy for productivity and for comparing relative productivity across rural production areas (FAO, 2015).

For transportation costs, the distance from the area to consumer centers was considered based on travel time using data from UNEP (UNEP, 2015) and ESA (ESA, 2008). Depending on the distance, a mode of transportation was chosen to serve the region (among truck, rail, and ship). Where distance ranges overlap, the average cost of these modes was considered. The combination of productivity factor and transportation cost was aggregated into seven sets of production costs. Thus, seven types of coverages were combined with seven cost categories.

For land use, there is a factor of total carbon content per area for each region and each type of cover. The calculation of emissions from land-use changes is made using this factor multiplied by the area deforested or planted, depending on its initial and final types.

Regarding the products from the agriculture sector, there are 25 in total (excluding other two bioenergy culture described below) as outlined in table 2.3. To calculate the demand for these products, a consumption value of kcal/hab/day is determined. This is based on historical data on how these kilocalories are distributed among the products in the table. The total values are then projected according to the population growth scenario of the narrative world scenario adopted in the simulation. The land use module treated cattle production separately due to its importance for supplying meat and milk and the extensive land use required for its husbandry in some parts of the world. Both for cattle production and agriculture (and each crop), a yield was assigned for each region in the model. Thus, for each product demand, there is a link to the amount of land needed to meet it. This method allows calculation of how much land is required to satisfy the production needs of specific agricultural products and livestock, taking into account regional variations in productivity.

Table 2.3: Agricultural products without bioenergy (Source: own elaboration based on (ROCHEDO, 2016))

CROPS						
Cereal	Coffee	Fiber	Fruits	Maize	Nuts	Oilseed
Pulses	Rice	Roots	Soybeans	Sugarcane	Vegetables	Wheat
PROCESSED CROPS						
Maize Oil	Soybean Oil	Sugar	Other Oil			
MEAT						
Bovine meat	Fish	Other Meat				
PROCESSED LIVESTOCK						
Animal fat	Butter	Eggs	Milk			

There are two other crops dedicated exclusively to energy production: woody biomass and grassy biomass. For these, there is also a production yield per cultivated area for each region. Additionally, in the biomass sector, various conversion technologies are addressed, each with its returns in terms of final products (ethanol, methanol, and biodiesel), and associated investment costs ($/kW) and O&M costs ($/kW/year). The possible conversions of crops to final energy products are described in table 2.4. This comprehensive approach allows for a detailed assessment of the potential and efficiency of different biomass types and their conversion technologies

2.2.2 TEA

Computable general equilibrium (CGE) modeling integrates economic theory with empirical data. These models simulate the market decisions of economic agents within resource allocation constraints. Figure 2.4 illustrates the circular flow of the economy, highlighting the main agents: households, firms and governments. Households supply production factors (labor, capital, and land) to the productive sectors. Firms demand these factors to produce goods and services. In return, firms pay households rents, salaries, and interest. Households then use this income to purchase goods and services, including investments. These transactions occur in the markets for factors of production and goods and services, respectively. Prices adjust

Table 2.4: Possible conversions of crops to biofuels in COFFEE

Ethanol	Sugarcane Corn Wheat Woody Grassy Beet Bagasse Residue
Methanol	Woody
Biodiesel	Soy Oil Maize Oil Animal Fat Oilcrops

to ensure that supply meets demand, achieving market equilibrium. Governments collect taxes and allocate their revenue towards consumption and direct transfers to households and firms. Economic agents make optimal choices regarding resource allocation based on their preferences, but these choices are constrained by factors such as disposable income, physical and technological availability, and the rules set by social and political institutions. The availability of resources influences the decisions made by these agents.

These models are valuable for policy analysis, helping to assess costs and benefits. They are commonly used to analyze overall welfare and measure the impacts of policies across multiple markets, including those related to taxes, subsidies, quotas, and transfer instruments.

According to the model documentation

> ”TEA (Total Economy Assessment) is a multi-regional and multi-sectorial CGE model that tracks the production and distribution of goods in a dynamic recursive setup for the global economy. The core equations and the static part of the model is based on GTAPinGAMS, while the recursive dynamic setup is based on the EPPA model. The model is formulated as mixed complementary problem (MCP) and is solved through Mathematical Programming System for General Equilibrium – MPSGE within GAMS. It assumes total market clearance, zero profit condition for producers and perfect competition to reach general equilibrium” (CUNHA *et al.*, 2020)

The model is based on microeconomic theory, in which consumers, subject to budget constraints, tend to maximize their well-being. Producers, on the other hand, aim to minimize total production costs given a certain level of technological development. TEA does not intend to investigate issues of tariff, budget, and potential economic policies for distribution improvements. Therefore, the government

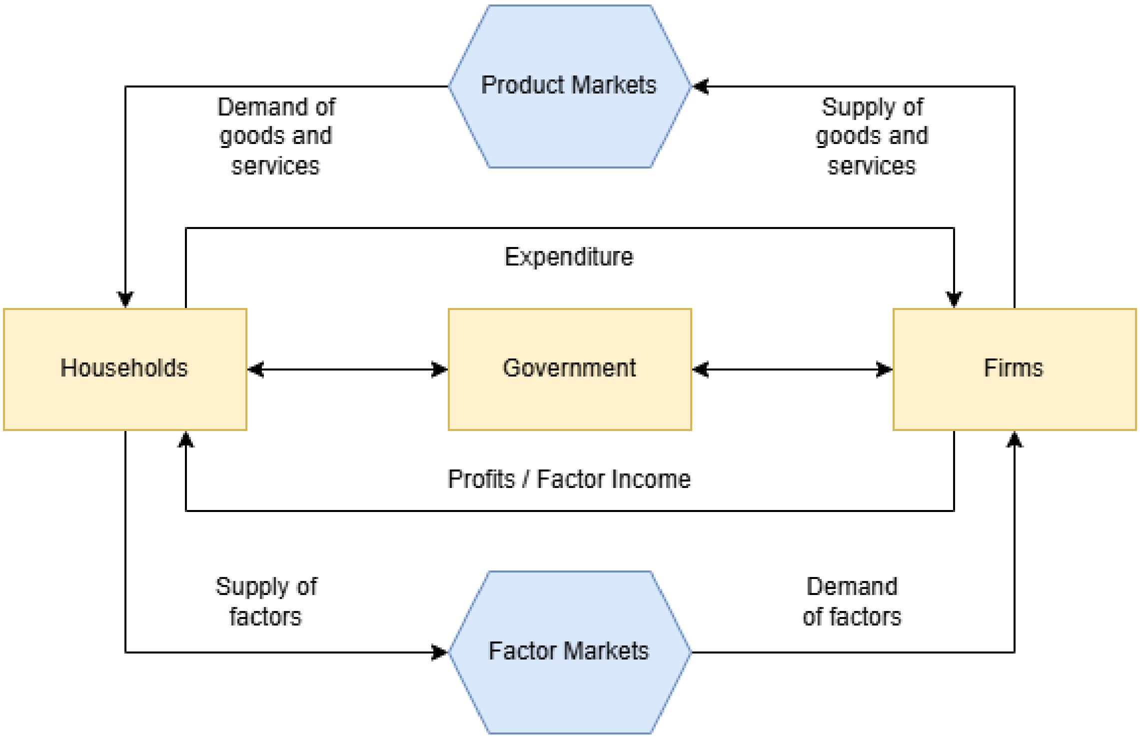


Figure 2.4: The economic circular flow into a CGE (Source: own elaboration)

(public agent) and families (representative private agent) have their representations unified. Exceptions to this rule include carbon dioxide tariffs and subsidies for carbon mitigation, as well as cap-and-trade policies and carbon budgeting strategies. These exceptions represent targeted interventions designed to address the externalities associated with carbon emissions.

The equilibrium conditions—market clearance, zero profit, and income balance—are briefly described below:

Market clearance refers to the condition where supply equals demand in every market within the economy. In other words, for every good and service, the amount that producers are willing to supply matches exactly with the amount that consumers are willing to purchase.

Zero profit in economic models, particularly those assuming perfect competition and constant returns to scale, refers to a situation where firms earn just enough revenue to cover their total costs, including opportunity costs. This means that in the long run, firms do not earn economic profits because any positive profits would attract new firms into the market, driving prices down until profits are zero. Zero profit equilibrium ensures that resources are allocated efficiently and no firm has an incentive to enter or exit the market.

Income balance pertains to the equilibrium condition where households allocate their income between consumption and savings (investment) in such a way that their utility is maximized. It means that households have optimally exhausted their income on goods, services, and savings such that their overall utility is at its highest possible level. In the context of the model, this implies that all income generated by households is either spent on consumption or invested, ensuring that there is no unutilized income.

Regarding time horizon and resolution, TEA starts in 2011, ends in 2100, and the calculation stages occur every five years. As for its regional division, since it is a model created to be integrated with COFFEE, it follows the same 18 regions as the associated IAM. Regarding sectors, it is divided into five macrosectors with their subdivisions as shown in table 2.5.

Regarding the factors of production, the model utilizes capital and labor as variable factors with intra-regional mobility, while land and natural resources are considered fixed factors. This distinction allows for the dynamic modeling of economic activities where capital and labor can respond to regional economic conditions and incentives, shifting across regions to optimize output and efficiency. Conversely, land and natural resources remain constant within each region, reflecting their inherent immobility and scarcity.

Table 2.5: Sectoral Aggregation of the TEA Model (Source: (DA CUNHA, 2019, p. 71))

Sector Groups	**Subsector Description**
Agriculture	Agriculture and forestry
	Cattle (beef, sheep, goats, and equine)
	Other animals (swine, poultry; also dairy, eggs, etc.)
	Fishing
Energy	Coal
	Crude oil
	Electricity
	Natural gas
	Petroleum products
Industry	Iron and steel
	Chemical and petrochemical
	Non-metallic minerals (cement, lime, concrete, etc.)
	Food industry without meat[3]
	Meat industry
	Other industries (mining, paper and pulp, etc.)
Transport	Land transport (road, rail, etc.)
	Water transport
	Air transport
Residential / Services	Commercial / Services
	Residential

TEA also accounts for emissions of CO_2, CH_4, and N_2O, categorized as emissions from the combustion of fossil fuels or emissions related to industrial processes, energy, and land use sectors. Non-CO_2 gas emissions are converted into CO_2 equivalent based on the Global Warming Potential for a 100-year horizon (GWP100).

The soft-link between COFFEE and TEA is facilitated through a demand generation module that reconciles differences between the sectoral divisions of the two models. In an initial round, having received the same macroeconomic inputs from the scenario to be run in COFFEE (e.g., SSP2), TEA provides COFFEE with data on sectoral demands and technological costs. COFFEE then uses these demands to meet them at the lowest cost and within imposed constraints. Subsequently, COFFEE provides TEA with the capacity for energy supply; the breakdown of this supply by type of source; technological progress; energy efficiency; and emission trends. This iterative process allows for integrated and dynamic interaction between the two models.

2.3 MFA

Mass Flow Analysis (MFA) is a systematic methodology used to quantify the flow of materials and energy within a defined system, typically over a specified period (BACCINI and BRUNNER, 1991). This method is fundamental in understanding the material metabolism of a system, allowing researchers to track the input, output, and accumulation of materials (stock formation). It operates on the principle of mass conservation, ensuring that the mass entering a system equals the mass leaving the system plus any changes in stock within the system (MÜLLER *et al.*, 2014), (BAARS *et al.*, 2022).

MFA is widely applied in various fields, including environmental science, industrial ecology (IE), and resource management. It helps in identifying inefficiencies, potential areas for improvement, and the environmental impacts of material flows. By mapping out the pathways and transformations of materials, MFA provides a comprehensive picture of the system's material dynamics, aiding in the development of strategies for sustainable resource use and waste reduction (PAULIUK *et al.*, 2017), (PAULIUK *et al.*, 2021a).

2.3.1 Simple MFA

A simple or static Mass Flow Analysis model is a snapshot of the flow of a certain material through a sequence of processes within a system over a specific time (MÜLLER *et al.*, 2014). There are some basic characteristics that must be defined in such a system (INDUSTRIAL ECOLOGY FREIBURG, 2018):

- **System Boundaries:** These define which processes and parts of the system are under study. Determining the boundaries is crucial as it delineates the scope of the analysis and ensures that all relevant processes involving the material are included.

- **Processes:** These are parts of the system where the element or material of study is transformed, distributed, or stored. Examples include the production phase of an ore or the usage phase of a material. Each process within the boundaries of the system must be clearly defined and understood in terms of its role in the material's lifecycle.
- **Stocks:** This refers to the storage of material or products that use the material under study. The stock is always linked to a process. For instance, considering the usage phase (process) of an element, such as iron, this material is stored for years in this process in the form of buildings, cars, appliances, among others. The stock represents a temporary resting place for materials within the system and can vary significantly in size depending on the material and process dynamics.
- **Flows:** These define the transitions from one process to another and can link them, for example, through yields. Recycling of a material is a flow that links the disposal phase or usage phase back to the manufacturing of that material.
- **Materials and Goods Analyzed:** This defines which materials will be studied and which manufactured goods using these materials will be addressed. A Mass Flow Analysis (MFA) can analyze more than one material at the same time, as well as their incorporation into various consumer goods.
- **Time Scope:** Analyzed time instant (static) or time interval (dynamic)
- **Spatial Scope:** Definition of the region that will be analyzed in the MFA, which could be, for example, a country or a continent. This aspect determines the geographical boundaries within which the material flows are quantified and assessed

Flows are critical for understanding how materials move through a system, their transformation, and eventual reuse or disposal. Is important to notice that flows always link one process to other, they never bifurcate.

In the given figure 2.5, a simple Mass Flow Analysis (MFA) system is depicted involving three processes, two of which involve stock formation. The system is described by an inflow, F_{01}, which enters the system boundaries, and two outflows, F_{20} and F_{30}. which exit from the second and third processes respectively. This kind of system can be analytically solved provided there is sufficient information about the flows and stocks. Equations that describe the system are found in equations 2.1, in which each F_{ij} represents a material flow between processes i and j, while ΔS_i is the stock formed in process i.

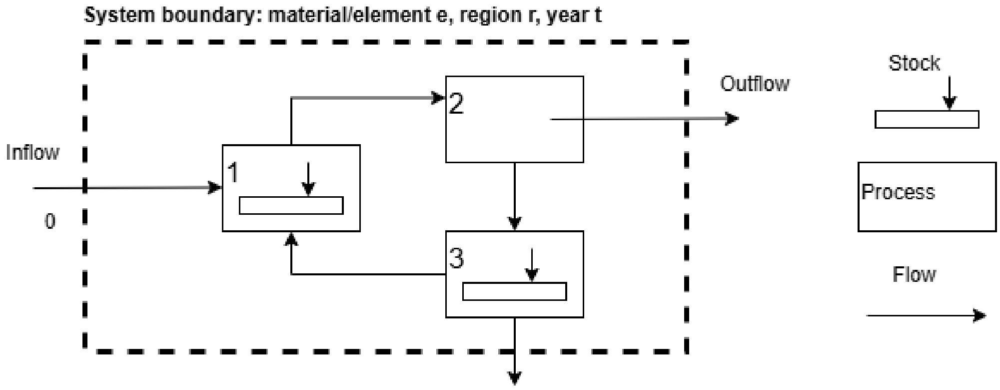


Figure 2.5: Example of a simple MFA system (Source: (INDUSTRIAL ECOLOGY FREIBURG, 2018))

$$
\begin{aligned}
\text{Process 1:}\quad & F_{01} + F_{31} - F_{12} = \Delta S_1 && \text{(2.1a)}\\
\text{Process 2:}\quad & F_{12} - F_{23} - F_{20} = 0 && \text{(2.1b)}\\
\text{Process 3:}\quad & F_{23} - F_{31} - F_{30} = \Delta S_3 && \text{(2.1c)}\\
\text{System:}\quad & F_{01} - F_{20} - F_{30} = \Delta S_1 + \Delta S_3 = \text{net inflow} && \text{(2.1d)}
\end{aligned}
$$

2.3.2 Dynamic MFA

To analyze more complex systems and variables, such as stock formation over time, consumption of a specific material, waste quantities, etc., an analysis that extends over time is necessary. Dynamic MFA (dMFA) has precisely this characteristic, where every variable becomes time-dependent. Thus, the equations in 2.1 would be modified to 2.2. The system boundaries now have a time interval, not just a single point in time.

$$
\begin{aligned}
\text{Process 1:}\quad & F_{01}(t) + F_{31}(t) - F_{12}(t) = \Delta S_1(t) && \text{(2.2a)}\\
\text{Process 2:}\quad & F_{12}(t) - F_{23}(t) - F_{20}(t) = 0 && \text{(2.2b)}\\
\text{Process 3:}\quad & F_{23}(t) - F_{31}(t) - F_{30}(t) = \Delta S_3(t) && \text{(2.2c)}\\
\text{System:}\quad & F_{01}(t) - F_{20}(t) - F_{30}(t) = \Delta S_1(t) + \Delta S_3(t) = \text{net inflow}(t) && \text{(2.2d)}
\end{aligned}
$$

Additionally, although the system is factually continuous, it is modeled as a discrete-time system as if sampled at a fixed period. This period is typically one year, the interval for which statistical databases are commonly compiled and published.

The figure 2.6 presents a model of a complete dynamic MFA (dMFA) cycle, ranging from mining to the disposal phase. A model does not need to address all the processes shown in figure 2.6; part of the modeling involves defining the processes (phases) that are covered.

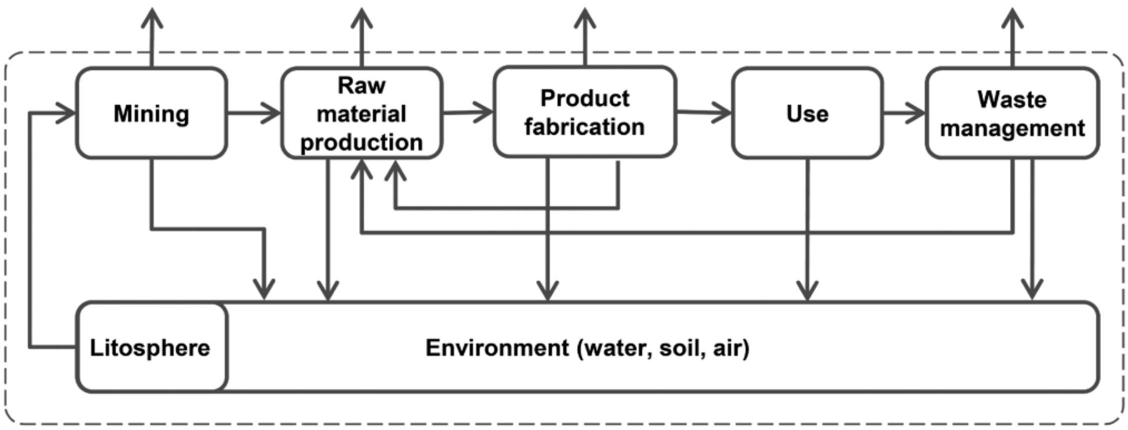


Figure 2.6: Generic dMFA model (Source: (MÜLLER *et al.*, 2014))

In the upcoming subsections, various aspects that define a dynamic MFA (dMFA) will be discussed. A summary of these is compiled in table 2.6 taken from (MÜLLER *et al.*, 2014). This table outlines the key components and parameters necessary for constructing a comprehensive dMFA model, providing a structured approach to analyzing material flows and stocks over time. The section is build mainly reproducing the same structure of analysis used by Müller (MÜLLER *et al.*, 2014).

2.3.2.1 Top-down and Bottom-up Approaches

There are two approaches to dynamic Material Flow Analysis (MFA): top-down and bottom-up. In the top-down approach, aggregated data are used, typically concerning the inflow into the system or the total available stock, as known variables. The variation in stock S within the system is calculated based on the net inflow using the mass balance principle. This approach can be numerically described by the formula 2.3 (MÜLLER *et al.*, 2014).

$$dS(t) = (\text{inflow}(t) - \text{outflow}(t)) \cdot dt = \text{net flow}(t) \cdot dt \tag{2.3a}$$

$$S[n] = (\text{inflow}[n] - \text{outflow}[n]) \cdot T + S[n-1] \tag{2.3b}$$

In which the first equation in 2.3 refers to the stock variation $dS(t)$ in continuous time t, and the second to the integrated form of the equation described in discrete time n.

For $n = N$, where N it's the final year of the model:

$$
\begin{aligned}
S[N] &= (\text{inflow}[N] - \text{outflow}[N]) \cdot T + (\text{inflow}[N-1] - \text{outflow}[N-1]) \cdot T + \ldots \\
&\quad + S[N-(N-1)] + S[0] \\
S[N] &= S[0] + T \cdot \sum_{n=1}^{N} (\text{inflow}[n] - \text{outflow}[n])
\end{aligned}
\tag{2.4}
$$

In the bottom-up approach to dynamic Material Flow Analysis (MFA), stocks are constructed by summing up the content c_i of the element/material/metal under investigation in each final product P_i. The stock in year n can then be calculated according to the equation 2.5. This method provides a detailed and granular analysis by accounting for how each component contributes to the overall stock, offering insights into the specific contributions and life cycles of materials within the system. It is especially useful for tracing specific materials through complex product chains and for evaluating the impacts of individual products on material stocks over time.

$$
S[n] = \sum_{i=1}^{I} P_i[n] \cdot c_i[n] \tag{2.5}
$$

2.3.2.2 Outflows as a Function of Inflows or Stocks

There is a common problem where input and stock data are available in databases, but outflows are not. The most commonly used approach to address this issue is to treat the outflow as a proportion of the inflow using the lifetimes of the final products. This is typically done using the same methods as in reliability engineering, where probability density functions (pdf) for the lifetimes of the final products are assigned. The supplementary material table from (MÜLLER *et al.*, 2014) provides the formulas, parameters, and a discussion of each of the six functions most commonly used in this field: Weibull, Delta, Normal, Lognormal, Beta, and Gamma. The outflow in a given period is the convolution of the inflow with the pdf according to equation 2.6, where the symbol "*" represents convolution [4].

$$
\text{outflow}(t) = (\text{inflow} * f)(t) = \int_{-\infty}^{\infty} \text{inflow}(t-\tau) \cdot f(\tau)\, d\tau \tag{2.6}
$$

Here, it is important to note that the goal is to find the outflow at a specific time t, however, the probability distribution $f(\tau)$ extends from $-\infty$ to ∞, which is the integration space of the convolution definition (see Annex I). At some point in the integration of equation 2.6, the time τ will be the same as t.

From a practical perspective, dynamic MFAs (dMFAs) are carried out discretely, databases are typically provided in discrete time periods, usually annualized. In this

[4] More about convolution can be found in Annex I

case, the convolution integral can be represented by the convolution sum given by the equation 2.7, where the time t is replaced by a discrete time n and the integrated variable τ is replaced by a discrete time m.

$$\text{outflow}[n] = \sum_{m=-\infty}^{\infty} \text{inflow}[n-m] \cdot f[m] \tag{2.7}$$

To better understand convolution in a dynamic MFA, consider the process represented in figure 2.7 to be a linear time-invariant system (LTI), that is, if the generic responses $o(t)$ to inputs $i_1(t)$ and $i_2(t)$ are $h_1(t)$ and $h_2(t)$ respectively, then for an input $i(t) = a \cdot i_1(t-\tau) + b \cdot i_2(t-\tau)$ the output will be $o(t) = a \cdot h_1(t-\tau) + b \cdot h_2(t-\tau)$ where a, b, and τ are constants.

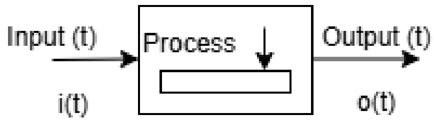
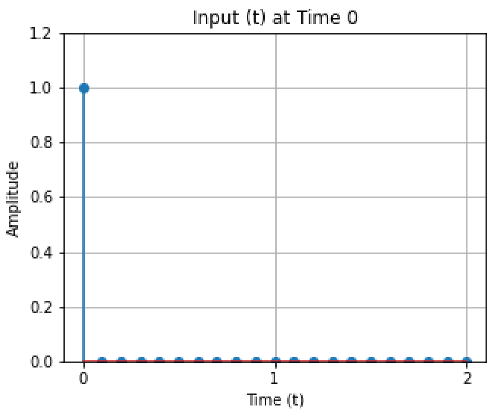
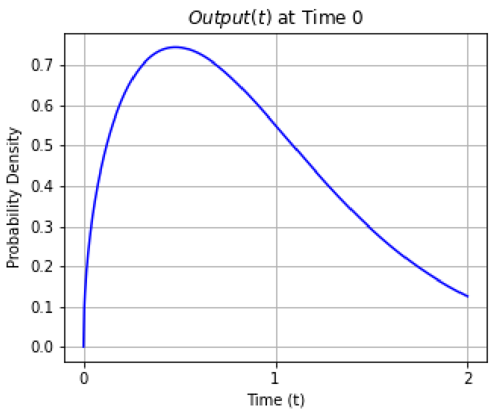


Figure 2.7: Example of a simple MFA system (Source: own elaboration)

The input is modeled as an impulse function (or Dirac delta function), but in reality, it is a function distributed over time (e.g., mass of copper in the system) which, for practical reasons previously discussed and due to ease of modeling, is described as such. Each input at a given time t will generate an output that gradually distributes over time. An example would be steel in the usage phase of automobiles; as time passes, part of this steel exits the usage phase (output) and enters another process, such as waste management. For equipment that has a predetermined lifespan, like devices that must be replaced at fixed intervals due to regulatory reasons, the output will be a time-shifted impulse. For the vast majority of final uses, the output will be a probabilistic distribution, as already mentioned.



(a) Impulse at time $t = 0$



(b) Impulse response at time $t = 0$

Figure 2.8: Impulse as input and it output response

Each input into the system at a given time t will generate an addition of a stock function that can be separated by its time t of origin and is called the age-cohort of t. Essentially, this output is the response to the impulse function (see Annex I) of the process, and, thinking about a dynamic MFA (dMFA), it would be the probability distribution function of the lifetime of a specific durable good [5]. This can be represented by figure 2.8a.

To give a practical example, still with automobiles, if we want to know the output of a system at time $t = 3$, considering a system that starts at $t = 0$, we must sum the product of the automobiles produced at $t = 0$ by the probability of the automobiles that entered at $t = 0$ having been discontinued by $t = 3$, and do the same for the automobiles that entered in use at $t = 1$, $t = 2$, and $t = 3$ (sudden death of a good).

The total output will then be the sum of series of responses to a series of inputs, that is, the sum of these age-cohorts, which are necessarily shifted in time. Figure 2.9 illustrates this situation.

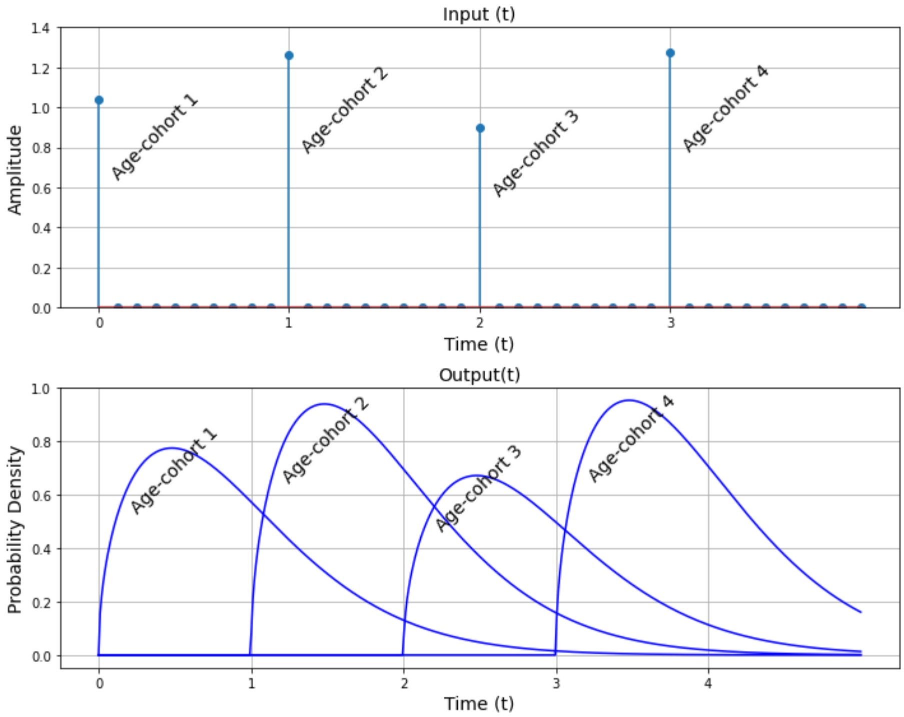


Figure 2.9: Age Cohorts: Input and Output

Every Δt in the discrete case is 1, so T=1. Inserting, for the continuous case, equation 2.6 into 2.4 or equation 2.7 for the discrete case, we derive the following equation for the total stock in year N:

[5] A global MFA would include many final uses, which would result in a response that is the summation of the different PDFs of the evaluated final-use goods

$$S[N] = S[0] + T \cdot \sum_{n=1}^{N} (\text{inflow}[n] - \int_{-\infty}^{\infty} \text{inflow}(t-\tau) \cdot f(\tau)\, d\tau)$$
$$S[N] = S[0] + \sum_{n=1}^{N} (\text{inflow}[n] - (\sum_{m=-\infty}^{\infty} \text{inflow}[n-m] \cdot f[m])) \tag{2.8}$$

The equation for the discrete case can also be obtained by the simple equation for stock variation $\Delta S(t) = I(t) - O(t)$:

$$S[N] = \sum_{0}^{N} \Delta S[t] = \sum_{0}^{N} I[t] - O[t]$$
$$S[N] = S[0] + \sum_{n=1}^{N} (\text{inflow}[n] - (\sum_{m=-\infty}^{\infty} \text{inflow}[n-m] \cdot f[m])) \tag{2.9}$$

Essentially, it involves summing all the inputs up to the year for which the stock is to be calculated and subtracting from this value the outputs calculated with the convolution in 2.7 and 2.6, as shown in Figure 2.10

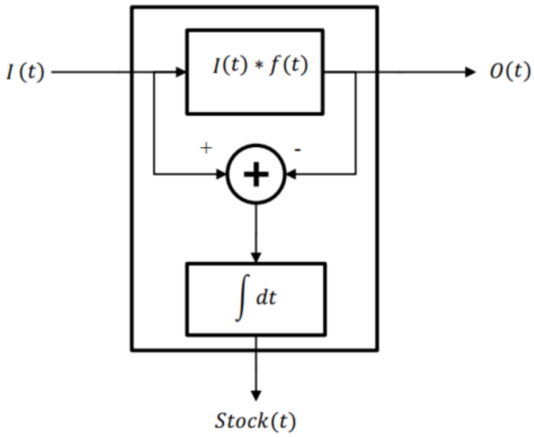


Figure 2.10: Stock flow diagram (Source: (MÜLLER *et al.*, 2014))

2.3.2.3 Stock and Input Driven

In addition to the categorization between top-down and bottom-up approaches, equations 2.8 and 2.9 suggest that the system can be developed based on known stocks (stock-driven) or known inputs (input-driven). Known inputs might include, for example, the time series of silicon consumption by the semiconductor industry or the annual production of copper. Known stocks could be the number of cars in circulation in a country or the estimated built-up area in a region.

2.3.2.4 Prospective and Retrospective

Another distinction is whether the system operates in the past (retrospective) or the future (prospective). As an example of retrospective use, in (MÜLLER *et al.*, 2006), Muller et al. quantify the amount of iron in use in the USA using, among other data, the country's steel consumption over the last century. Another example is in (LIU and MULLER, 2013), which analyzes past flows to understand the position of certain countries in the aluminum chain, from extraction to the usage phase. In (ZUSER and RECHBERGER, 2011), there is an example of a prospective study, in which the demand for materials for four different types of PV technologies is analyzed. Common studies combine both perspectives. This occurs because past data influence or are used to project scenarios, demands, inputs, and future stocks.

There are various ways to construct future perspectives of stocks and inputs. Generally, parametric equations are used that relate material inputs and stock growth to other quantities like GDP, population, technological development, among others. The level of complexity can vary; in (VAN BEERS and GRAEDEL, 2004) the projection of future stock has time as the only independent variable, assuming that future growth will follow past trends. In (ELSHKAKI *et al.*, 2016), future copper demand depends on time and the region's per capita GDP. In (NORTHEY *et al.*, 2014), the future global demand for copper has a relationship with the evolution of reserves and follows a Hubbert curve model.

Some studies where future projections are more complex to trace include (DEETMAN *et al.*, 2018), where the demand for copper, tantalum, neodymium, cobalt, and lithium for electricity generation technologies, cars, and electronic appliances is estimated from data from the Integrated Model to Assess the Global Environment (IMAGE), and each use has a different approach. In the case of cars, for example, a certain amount of stock in use is necessary for the transport service in pkm to be met. In this sense, data such as kilometers driven annually, average occupancy rate, fleet in the initial year, and statistical distribution of the fleet's usage time are necessary. For appliances, population, income, housing, and people per household were used. In (DEETMAN *et al.*, 2021), outputs from the IMAGE's energy generation for SSP2 scenarios were used to estimate the consumption of materials such as steel, aluminum, and neodymium. In this case, a projection of equipment to meet such production was made, and in a bottom-up approach that considers the mass of these materials per piece of equipment, the total demand in a future scenario is estimated.

2.3.2.5 Dissipation

During the lifecycle of a material, each process may involve dissipation, which are losses to the environment, i.e., outputs outside the system boundaries, as illustrated in figure 2.6. Examples of this dissipation include non-reusable metal filings during the production phase, losses due to corrosion and abrasion wear during the usage phase, and small percentages of metal in alloys that are discarded when recycling, prioritizing the main metal, among others. There are several ways to account for this dissipation. One method is through mass balance, if data are available. Another method is to consider fixed loss factors per process. A third method varies these same factors over time, considering process efficiency improvements in the future. Dissipation can also be categorized as intentional or unintentional. For example, intentional dissipation may include materials that are discarded after the use phase because they are not economically viable to recycle, while corrosion could be considered unintentional dissipation.

2.3.2.6 Spatial Resolution

The previous section, Simple MFA, discussed the need for defining the spatial boundary of the system. Additionally, within the system, multiple regions can be established, similar to what is done in IAMs. As will be seen later when discussing the ODYM, the division into regions will establish an additional dimension in the system's vectors. A durable good, such as buildings, for example, can be modeled as a vector where there is the mass content of steel and cement, which constitutes a dimension of size 2, referring to two materials; if it spans from 2011 to 2060, it will have a second temporal dimension of size 50, one for each year; if divided into 5 regions, it will have a third dimension of size 5, one for each region. Thus, the data at position 1:10:2 would be, for example, the quantity of steel per square meter in a construction in the year 2021 in South America (assuming this is the region in position 2).

2.3.2.7 Uncertainty

Dynamic MFA models can also take into account uncertainty. This is important because there is imprecision in databases, and as (SCHNEIDER and MOSS, 1999) notes, this imprecision increases further along in the material cycle (see figure 2.6). Thus, there is more certainty about data on the production of pure copper than about its collection for recycling. In (MÜLLER *et al.*, 2014), four ways of dealing with uncertainty in MFA studies are mentioned. The first is simply not addressing it. The second involves conducting sensitivity analyses by changing parameters of the lifespan distribution, material intensity in production, and the factors of utilization and losses. A third method is to work with confidence intervals. Lastly, a fourth method involves error propagation using the Gaussian method, which will not be addressed here.

2.3.2.8 Input data

The input data in a dynamic MFA (dMFA) vary depending on several factors, including the approach, level of complexity, available data, analyzed processes (see figure 2.6), the quantity of materials and minerals considered, the number of consumer goods taken into account, and the environmental aspects analyzed. For example, in (DEETMAN *et al.*, 2020), the demand for steel, aluminum, and cement, as well as their stocks for residential and service buildings globally up to 2050, is forecasted. For this model, data such as the intensity of these materials per m2 of built area for each type of construction were needed; the amount of built area already present (year the simulation starts); the probability distribution and its parameters for the lifespan of each type of construction; the distribution of the lifespan of buildings at the present time; the average occupancy rate of each residence; population projections until the end of the model; the link between GDP and built area for constructions in the service sector; and the GDP growth perspective. All these variables are exogenous to the model, serving as inputs (population growth projections) or configuration parameters (e.g., material intensity per m2 of built area).

Another example, in (GLÖSER *et al.*, 2013), a retrospective analysis of the entire copper cycle is conducted. This analysis uses data such as mining and annual copper production; losses and reuses in production; copper intensity for various end uses (plumbing, industrial motors, household applications, etc.); material collection rates for recycling; and recycling yields, among others.

Collecting this type of data is exhaustive and often depends on estimates. As previously discussed, the further one advances in the material cycle, the greater the uncertainty. Common databases for consulting this data include industrial associations, UN statistics, national agencies such as the USGS, Eurostat, various reports from international institutions like the World Bank and NGOs, scientific articles, etc.

2.3.2.9 Output data

The output data depend on the model's objectives and the known input data. As previously mentioned, it is possible to investigate the current stock of a specific material, its future demand, recycling rates, among other aspects.

2.3.2.10 Initial conditions

When the model begins describing stock formation, it typically assumes a null stock at $t = t_0$ if it refers to a more distant period, when the consumption and stocks of a particular material were minimal compared to current levels (MÜLLER *et al.*, 2014). Occasionally, updated stock data are available to the modeler, and the year $t = t_0$ is a year closer to the present. In these situations, in a more simplified approach, the initial year receives an input that sums up the entire stock mass. In more sophisticated approaches, this stock is built up more gradually in the years preceding the $t = t_0$ of interest.

2.3.2.11 Evaluation

Although Müller (MÜLLER *et al.*, 2014) considers this aspect as part of the model, it is understood that evaluating the results goes beyond its construction. The same result can be interpreted, explored, and condensed in different ways by different authors. However, as will be discussed later in the description of ODYM, certain models allow for the evaluation of additional aspects beyond the traditional scopes of a dMFA. For example, ODYM-RECC v2.5 includes analyses of environmental impacts such as GHG emissions and water use at certain stages of the material cycle (PAULIUK, 2023).

Table 2.6: Overview, Design Concepts and Details Protocol for MFA, (Source: (MÜLLER *et al.*, 2014))

Overview	**Purpose**	What is the purpose and general framework of the model?
	Materials (goods, substances)	What materials (goods/substances) are included? Are materials further divided into material categories (and subcategories)?
	Processes	What processes are included? Do they transform, transport, or store materials? Are processes further divided into process categories (and subcategories)?
	Spatial and temporal scale and extent	What is the spatial and temporal scale and extent of the study?
	System overview	What is the structure of the system regarding processes, stocks, and flows?
Design concepts	**Basic principles**	Static or dynamic, top–down or bottom–up, retrospective or prospective?
	Static or dynamic modeling approaches	How are stocks and flows modeled? What are the extrapolation methods for exogenous variables?
	Dissipation	How does the model account for dissipation?
	Spatial dimension	How does the model account for the spatial distribution of stocks and flows?
	Uncertainty	How does the model account for data and model uncertainty?
Details	**Initial condition**	How is the initial state (e.g., the initial stocks and flows) of the model set?
	Model input data	What data is used as input to the model?
	Model output data	What data is generated as model output?
	Evaluation	What methods (e.g., for data aggregation and visualization) are used to evaluate the results?
	Detailed model description	What, in detail, is the formal description (e.g., equations) of the system and what are the algorithms (e.g., solution procedures) used for the calculations? What are exogenous and endogenous model variables? What are the model parameters, their dimensions, and reference values?

2.4 ODYM-RECC

In the upcoming sections, the following will be described: the framework for dMFA provided by ODYM, the RECC strategy, and the potential contributions of integrating the first two with IAMs. The first one is based on ODYM documentation available in it's GitHub Wiki and in PAULIUK and HEEREN (2020b). The second one is based on RECC documentation available in PAULIUK (2023).

2.4.1 ODYM

The ODYM was developed to address a recognized gap within Industrial Ecology (IE) methods. According to Pauliuk and Heeren (PAULIUK and HEEREN, 2020b), MFAs are typically conducted by isolated groups of researchers, software used are not open-source, are poorly documented, and often not peer-reviewed. The development of ODYM aims to create a transparent and collaborative environment, written in Python code and openly available on the GitHub platform at (https://github.com/IndEcol/RECC-ODYM). Each version of the software is accompanied by documentation of features and aggregated data, as well as scientific materials produced from them (INDUSTRIAL ECOLOGY FREIBURG, 2024b). It has a data structure that allows archiving, exchanging and re-using data.

2.4.1.1 ODYM framework and principles

Beyond the software, ODYM serves as a dMFA framework due to its structure, which includes rigidity in fundamental aspects and flexibility for adaptation to various situations, studies, and flows. In PAULIUK and HEEREN (2020b) the rigidity and flexibility of each of the following aspects are evaluated:

System definition: When building a model, the system definitions are rigid; the processes are defined (take definitions from section 2.3.1 and figure 2.6), for example, mining, manufacturing of engineering materials, manufacturing of consumer goods, usage phase, among others. This definition remains static after being set in ODYM. However, there is flexibility at the time of definition and during the use of the system. Processes can be added or removed during the definition phase. Moreover, the processes are multi-layered; the usage phase can include the various final products evaluated, and the manufacturing phase of engineering materials can include multiple manufacturing processes. Figure 2.11 illustrates these definitions for ODYM-RECC v2.4. During software manipulation, for calculations and results display, items can be shown individually or aggregated. Items follow the hierarchy of the process, inheriting its characteristics defined by the aspects (addressed next).

Classification: All aspects of the system, such as regions, age-cohorts, materials,

Name	Ores_RawMaterials_m1	Material_Production_i2	Engineering_Materials_m2
Dimension	Material	Process	Material
Description	List of ores and raw materials, extracted in primary production sector	List of producers of engineering materials (in the narrow sense)	Lists of engineering materials (in the narrower sense), output of enginee
ID	None	None	None
UUID	80d6cda1-9451-4bc5-859e-e3a9c465453c	b8763818-37cc-4c81-823c-fac0c840dbac	0d06154b-ecf9-4e98-9379-8f030203ec00
Date created	18/11/2017	18/11/2017	18/11/2017
Last modified	18/11/2017	29/01/2019	23/07/2018
Last modified	Stefan Pauliuk	Stefan Pauliuk	Stefan Pauliuk
Reference	0	0	0
Items			
0	Limestone	cement plant (limestone)	construction grade steel
1	Iron ore	cement from ash or slag	automotive steel
2	Bauxite	pig iron production (blast furnace)	stainless steel
3	Oxidic copper ores	direct iron ore reduction	cast iron
4	sulfidic copper ores	BOF route steel making and remelting	wrought Al
5	Nickel ore	EAF route steel making and remelting	cast Al
6	Timber	iron foundries	copper electric grade
7	Crude oil	ferrocromium production	copper lower grade
8	Natural gas	ferromanganese production	plastics
9		ferronickel production	paper and cardboard
10		primary al production	cement

Figure 2.11: Partial screenshot of model definition in Classification_Master used in ODYM - Processes (Source: (PAULIUK *et al.*, 2021b))

goods, etc., follow a classification that is rigid concerning their dimensions (units). Dimensions are root categories within ODYM and can include time, element, material, process, region, energy carrier, scenario, good product, extension, and unity. Flexibility is within aspects, different aspects can share the same dimensions; for example, model year and age-cohorts both have the time dimension; vehicles and buildings fall under the Good product dimension; and production materials and engineering materials fall under the material dimension. Each aspect can have various items, as previously described. For instance, the "chemical elements" aspect could encompass the entire periodic table or just one metal. The processes that define the system are part of the aspects, and like them, other aspects are also contained in the Classification_Master table. Figure 2.12 provides another excerpt from the mentioned table showing other aspects.

Name	Chemical_Elements	SSP_Scenarios	RCP_Scenarios	SSP_Regions_11	Products_m3
Dimension	Element	Scenario	Scenario	Region	Good_Product
Description	100 first chemical elements, plus total	List of SSP Scenarios	List of RCP Scenarios	11 Regions for shared socioeconomic pathways (SSPs)	List of manufactured and constructed products
ID	None	None	None	None	None
UUID	ec0551bc-69f4-42fe-9725-65ed578e	8d6bab0f-6202-49d9-8cbf-ffca46c3	f474fc58-d503-414b-974f-aacfd6ddd	0d393633-cf2e-4e8b-b409-6a2070806d99	cccc83dd-4fea-4c46-ac8d-b1cca05e0602
Date created	20/10/2017	20/10/2017	01/06/2018	43671	20/10/2017
Last modified	23/07/2018	17/04/2019	01/06/2018	43671	08/05/2020
Last modified	Stefan Pauliuk	Stefan Pauliuk	Stefan Pauliuk	Stefan Pauliuk	Stefan Pauliuk
Reference	0	https://tntcat.iiasa.ac.at/SspDb/dsd?A	https://tntcat.iiasa.ac.at/SspDb/dsd?A	https://tntcat.iiasa.ac.at/SspDb/dsd?Action=htmlpage&page=about	0
Items					
0	All	LED	Baseline(unmitigated)	AFR	Internal Combustion Engine, gasoline (ICEG)
1	H	SSP1	RCP2.6	CPA	Internal Combustion Engine, diesel (ICED)
2	He	SSP2	RCP3.4	EEU	Hybrid Electric Vehicles (HEV)
3	Li	SSP3	RCP4.5	FSU	Plugin Hybrid Electric Vehicles (PHEV)
4	Be	SSP4	RCP6.0	LAC	Battery Electric Vehicles (BEV)
5	B	SSP5	RCP8.5	MEA	Fuel Cell Vehicles (FCV)
6	C			NAM	busses, diesel
7	N			PAO	busses, electric
8	O			PAS	motorcycles, gasoline
9	F			SAS	motorcycles, electric
10	Ne			WEU	light cargo trucks, diesel
11	Na				light cargo trucks, electric
12	Mg				freight trucks, diesel
13	Al				freight trucks, electric
14	Si				passenger trains, diesel

Figure 2.12: Partial screenshot of model definition in Classification_Master used in ODYM - Aspects (Source: (PAULIUK *et al.*, 2021b))

The list of items within an aspect may not be fully utilized, as will be seen later with the specification of the IndexTable. Moreover, in the same IndexTable, the dimensions of the vectors for each aspect are defined. The usage phase aspect will have a good products dimension with the quantity of final products evaluated by the dMFA. It may also include, for example, usage regions, production regions, and age-cohorts; this way, it is possible to specify how many cars were produced in the year 2030 in Latin America and are in use in the same continent. These dimensions (n regions, g goods, etc.) will be used to define the size of the multidimensional vector that will store each piece of data read from the database provided to ODYM.

Data Structure: The parameters, data, aspects, processes, among others, will follow a fixed data structure that, once established, cannot be changed, although the data itself can be modified or added. ODYM is provided with an xlsx configuration file that contains several tables, including: general information, which contains the model name, version, scope, and other basic data; the software version, which includes the version of ODYM used; the IndexTable, where the aspects are determined, and a section from the one used in RECC v2.4 is reproduced in figure 2.13; the list of processes, as shown in figure 2.14; and the list of parameters, as shown in 2.15. Other configuration tables may be provided, such as the model execution control table and the output control table (e.g., whether to plot graphs or not).

Index Table		(Time, element, and unity aspects must always be defined)			
Aspect	Description	Dimension	Classification	Selector*	IndexLetter (unique!)
Time	Model time	Time	Time	[315:361)	t
Cohort	age-cohorts	Time	Time	[200:361)	c
Element	chemical elements	Element	Chemical_Elements	[0,6,13,24,26,29,30,101]	e
Unity	trivial classification, 1 entry only	Unity	Unity	all	u
Region32	region of process or stock, region of origin (flow	Region	SSP_Regions_32	[2,13,31,32,33,34,35,36,37	r
Region11	region of process or stock, region of origin (flow	Region	SSP_Regions_11	all	l
Region5	region of process or stock, region of origin (flow	Region	SSP_Regions_5	all	f
Region1	region of process or stock, region of origin (flow	Region	SSP_Regions_1	all	o
MaterialProductionProcess	Engineering material production processes	Process	Material_Production_i2	[21,22,23,24,25,26,27,29,3	P
Engineering materials	Engineering materials considered	Material	Engineering_Materials_m2	[0,1,2,3,4,5,6,8,10,11,12,1:	m
ManufacturingProcess	Manufacturing processes	Process	Manufacturing_i3	[0,1,2,3,4,5,22,23,24,25,26	F
Sectors	Aggregated product groups (sectors) such as bui	Good_Product	Sectors	[0,2,4,6,7]	G
Good	List of ALL goods and products considered	Good_Product	Products_m3	[0,1,2,3,4,5,22,23,24,25,26	g
Cars	List of car types considered	Good_Product	Sectors_cars	all	p
OtherVehicles	List of other vehicles considered	Good_Product	Sectors_othervehicles	all	v
ResidentialBuildings	List of residential building types considered	Good_Product	Sectors_resbuildings	[0,1,2,3,4,5,6,7,8,9,10,11,1	B
NonresidentialBuildings	List of nonresidential building types considerec	Good_Product	Sectors_nonresbuildings	[24,25,26,27]	N
Infrastructure	List of infrastructure considered	Good_Product	Sectors_infrastructure	all	i
Industry	List of industry considered	Good_Product	Sectors_industry	all	I
Appliances	List of appliances considered	Good_Product	Sectors_appliances	all	a
WasteManagementIndustries	Waste management industries	Process	Waste_Mgt_Industries_i5	[18:28)	W
Waste_Scrap	waste and scrap types considered	Material	Waste_Scrap_m5	[0,1,5,7,8,11,14,20,26,30]	w
Energy	Energy consumed	Energy carriers	Energy_Carriers_m6	[0,2,6,8,9,10,11,13]	n
Scenario	Scenerios considered (e.g., SSP)	Scenario	SSP_Scenarios	[0,1,2]	S
Extensions	Costs, emissions factors, social impacts	Extensions	Process_Extensions	[0,1,2,3,4,11]	X
Scenario_RCP	RCP scenarios	Scenario	RCP_Scenarios	[0,1]	R
SSP_Population_model	Population model used for SSP scenarios	Scenario	SSP_Population_Models	[0]	M
ServiceType	Different uses of building energy: heating, cooli	Extensions	ServiceTypes	[0,1,2,5]	V
Archetype	Product archetypes	Good_Product	Product_Archetypes	all	A
Custom	Custom aspect, for calibration parameter	Unity	Custom	[0,1,2,3]	C
Car_segments	Segments of passenger vehicles	Good_Product	Segments_cars	all	s
Regions32goods	List of goods with regional aggregation level 32	Good_Product	Regions_32_goods	[0:19)	T
Regions11goods	List of goods with regional aggregation level 11	Good_Product	Regions_11_goods	all	L
Regions1goods	List of goods with regional aggregation level 1	Good_Product	Regions_1_goods	all	O
vironmental impact/pressure categ	Pressure indicator dimensions such as GWP etc.	Extensions	Env_midpoints	[1]	x

Figure 2.13: Screenshot of the RECC's Index Table (Source: (PAULIUK *et al.*, 2021b))

Workspace Structure: To run ODYM with the model configured by the modeler, it is mandatory to designate a reference folder in which the database, configuration tables, and ODYM libraries will be stored. This folder is also where the results and logs will be saved.

Process Group List		
Process Group Number	Process group name	Process type
0	Environment	environment
1	Mining and extraction	industry/transformation/storage
2	Ore markets	market/distribution
3	primary material production	industry/transformation/storage
4	market for primary materials	market/distribution
5	fabrication and manufacturing industries	industry/transformation/storage
6	market for consumer goods, buildings, vehicles,	market/distribution
7	use phase	industry/transformation/storage
8	EoL products distribution	market/distribution
9	waste management and remelting industries	industry/transformation/storage
10	waste and scrap markets	market/distribution
11	Obsolete stocks	industry/transformation/storage
12	secondary material markets	market/distribution
13	landfills	industry/transformation/storage
14	final disposal distribution	market/distribution
15	energy and servie supply	industry/transformation/storage
16	energy markets	market/distribution
17	remanufacturing_reuse	industry/transformation/storage

Figure 2.14: Screenshot of the RECC's Processes List (Source: (PAULIUK *et al.*, 2021b))

	Model Parameters						
No.	Process	Parameter_Name	Description	Version	Index structure	Aspect order	Layer selection
0	external	2_P_RECC_Population_SSP_32R	exogenous popula	V2.2	MtrS	[0,1,2,3]	[0]
1	use phase	2_S_RECC_FinalProducts_2015_passvehicles	in-use stock by age	V1.3	tcpr	[0,1,2,3]	[0]
2	use phase	2_S_RECC_FinalProducts_2015_resbuildings	in-use stock by age	V1.2	tcBr	[0,1,2,3]	[0]
3	use phase	2_S_RECC_FinalProducts_2015_nonresbuildings	in-use stock by age	V1.0	tcNr	[0,1,3,2]	[0]
4	use phase	1_F_Function_Future	service flows provi	V1.2	GrtS	[0,1,2,3]	[0]
5	use phase	1_F_RECC_FinalProducts_appliances	future in-use stock	V1.0	ocSRa	[0,1,2,3,4]	[0]
6	use phase	1_F_RECC_FinalProducts_industry	future and past inf	V1.0	ISRIc	[0,1,2,3,4]	[0]
7	use phase	2_S_RECC_FinalProducts_nonresbuildings_g	future and past in-	V1.0	Nc	[0,1]	[0]
8	use phase	2_S_RECC_FinalProducts_Future_resbuildings	future in-use stock	V2.3	StGr	[3,2,0,1]	[0]
9	use phase	2_S_RECC_FinalProducts_Future_resbuildings_M	future in-use stock	V1.0	GoS	[0,1,2]	[0]
10	use phase	2_S_RECC_FinalProducts_Future_NonResBuilding	future in-use stock	V1.0	GrtS	[0,1,2,3]	[0]
11	use phase	2_S_RECC_FinalProducts_Future_nonresbuilding	future in-use stock	V1.0	GoS	[0,1,2]	[0]
12	use phase	3_EI_Products_UsePhase_passvehicles	energy intensity of	V1.2	cpVnrS	[0,1,2,3,4,5]	[0]
13	use phase	3_EI_Products_UsePhase_resbuildings	energy intensity of	V1.3	cBVnrS	[0,1,2,3,4,5]	[0]
14	use phase	3_EI_Products_UsePhase_nonresbuildings	energy intensity of	V1.0	cNVnrS	[1,4,5,0,3,2]	[0]
15	use phase	3_IO_Vehicles_UsePhase	intensity of operat	V2.3	VrtS	[0,1,2,3]	[0]
16	use phase	3_IO_Buildings_UsePhase_Historic	intensity of operat	V1.3	cBVrS	[0,1,2,3,4]	[0]
17	use phase	3_IO_Buildings_UsePhase_Future_Heating	intensity of operat	V1.0	GrtS	[0,1,2,3]	[0]
18	use phase	3_IO_Buildings_UsePhase_Future_Cooling	intensity of operat	V1.0	GrtS	[0,1,2,3]	[0]
19	use phase	3_IO_NonResBuildings_UsePhase	intensity of operat	V1.0	cNVrS	[0,3,4,2,1]	[0]
20	use phase	4_TC_ResidentialEnergyEfficiency_Default	Transfer coefficien	V1.0	VRrnt	[0,1,2,3,4]	[0]
21	use phase	4_TC_ResidentialEnergyEfficiency_Scenario_Hea	Transfer coefficien	V1.0	VRrntS	[0,1,2,3,4,5]	[0]
22	use phase	4_TC_ResidentialEnergyEfficiency_Scenario_Cool	Transfer coefficien	V1.0	VRrntS	[0,1,2,3,4,5]	[0]
23	use phase	6_MIP_VehicleOccupancyRate	passenger vehicle	V1.3	GrtS	[0,1,2,3]	[0]
24	use phase	3_LT_RECC_ProductLifetime_passvehicles	lifetime of passen	V3.1	pr	[0,1]	[0]
25	use phase	3_LT_RECC_ProductLifetime_resbuildings	lifetime of resider	V4.2	Brc	[0,1,2]	[0]
26	use phase	3_LT_RECC_ProductLifetime_NonResbuildings	lifetime of nonresi	V1.0	Nrc	[0,1,2]	[0]
27	use phase	3_LT_RECC_ProductLifetime_appliances	lifetime of appliar	V1.0	a	[0]	[0]
28	use phase	3_LT_RECC_ProductLifetime_industry	lifetime of industr	V1.0	I	[0]	[0]
29	use phase	3_LT_RECC_ProductLifetime_nonresbuildings_g	lifetime of non res	V1.0	Noc	[0,1,2]	[0]
30	use phase	3_MC_RECC_Vehicles	material composit	V1.1	cmpr	[0,1,2,3]	[0]
31	use phase	3_MC_RECC_Buildings	material composit	V1.2	cmBr	[0,1,2,3]	[0]
32	use phase	3_MC_RECC_NonResBuildings	material composit	V1.0	cmNr	[0,1,2,3]	[0]
33	use phase	3_MC_RECC_Nonresbuildings_g	material composit	V1.0	mN	[0,1]	[0]
34	use phase	3_MC_RECC_industry	material composit	V1.1	Im	[0,1]	[0]
35	use phase	3_MC_RECC_appliances	material composit	V1.1	oam	[0,1,2]	[0]

Figure 2.15: Partial screenshot of the RECC's Parameters List (Source: (PAULIUK *et al.*, 2021b))

Generally, the workflow can be schematized in figure 2.16. The pre-analytical phase consists of data collection, model scope definition, among others. Modeling begins with the definition of aspects, for which there must necessarily be a definition of dimensions and their classification. Within the "Data Structure" space, metadata allow for version control, traceability of origin, modifications, and assumptions of the data used [6].In the system structure part, the scope of time, regional areas, and analyzed materials are defined. Additionally, some of the declared aspects are processes of the dMFA model, which are also included in the system definition. These processes will be interconnected by flows and may allow for the formation of stocks. Parameter variables, initial stocks are provided by the database collected in the pre-analytical phase. The IndexTable compiles data and structure and serves to configure the model whose configuration function, msc.MFAsystem, has the IndexTable as one of its initialization parameters.

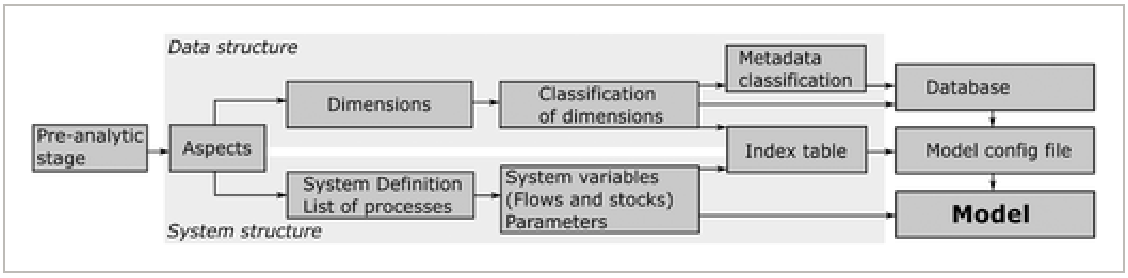


Figure 2.16: ODYM data model structure (Source: PAULIUK and HEEREN (2020b))

2.4.1.2 ODYM classes and functions

ODYM is based on an object-oriented code structure, so the definition of classes is crucial. It has three types of classes available in `ODYM_Classes.py` in its GitHub repository. The first class is where the system will be defined, the MFAsystem class, with the following attributes: index table, process list, stock dictionary, flow dictionary, parameter dictionary. The methods of this class include: Consistency check, mass balance check, data reformatting, and data export.

The second category of available classes is for the definition of processes, flows, stocks, and parameters. Each of these classes will have its necessary attributes; a flow, for example, will require parameters for the initial and final processes. The set of objects from this class will be grouped into lists or dictionaries [7] and will serve as attributes for the MFAsystem class that defines the system.

[6]Further guidelines for this can be found in `https://www.industrialecology.uni-freiburg.de/research/Documents/ODYM_Data_Processes_ODP_Manual.pdf`

[7]For a precise definition of lists and dictionaries in Python, check the official documentation at https://docs.python.org/3/tutorial/datastructures.html

Finally, the third category of classes includes those for auxiliary calculations, data reading, and also used during the execution of certain methods.

2.4.1.3 Using `einsum` in Multidimensional Array Operations

The `einsum` function in NumPy provides a powerful and flexible way to perform various array operations by leveraging Einstein summation convention. This function is highly beneficial for complex multidimensional data manipulations due to its concise syntax and efficient computation. Below, we illustrate the advantages of using `einsum` with two examples relevant to the subject.

Example 1: Aggregating Multidimensional Data: Suppose we have a multidimensional array A that carries data on the chemical content of end-use products. The dimensions (given by the aspects in the IndexTable in figure 2.13) of A are as follows: e is the number of chemical elements; m the engineering materials (e.g., steel, electrical grade copper, cement); r the regions; and g the list of final products or good. To simplify this data by aggregating the engineering materials dimension, we can use the `einsum` function as follows:

```
A_simplified = np.einsum('emrg->erg', A)
```

This operation effectively sums over the engineering materials dimension (`m`), resulting in an array $A_{\text{simplified}}$ with dimensions (e, r, g). The `einsum` function provides a clear and concise way to perform this aggregation, enhancing readability and maintainability of the code.

Example 2: Replicating Data Across Dimensions: Another example, used in the RECC, is when one wants to replicate the energy intensity of a vector for different scenarios, thus avoiding inserting columns with identical values in the data input table. For instance, the vector 'EI_UP_rbuild' (Energy Intensity of residential buildings during the use phase) was provided for only one Radiative Concentration Pathway (RCP) scenario. These intensities will be the same for all RCPs and have the dimensions c, B, V, n, r, and S (see IndexTable in figure 2.13). The operation below adds another dimension relative to the number of RCP scenarios used, reproducing the data for both, where `np.ones(NR)` is a unit vector of dimension NR (number of RCP scenarios).

```
EI_UP_rbuild = np.einsum('cBVnrS,R->cBVnrSR',EI_UP_rbuild,np.ones(NR))
```

2.4.1.4 Modeling a dMFA into the ODYM framework

The construction of a dMFA model within ODYM is located in the "Project Domain" depicted in figure 2.17. As previously discussed, there is an Excel configuration file for the model (project). This file includes basic data, a list of used aspects, the IndexTable, a list of parameters, a list of processes, script execution options, and output control. The reading of these parameters is automated by the script as long as the spreadsheet's formatting remains unchanged. Another spreadsheet, the classification sheet (Classification_Master), contains a list of all possible aspects that can be used within the project, along with their items. For example, as shown in figure 2.12, there are two "scenario" aspects, the SSP_scenarios and the RCP_scenarios; one may choose to list only one of them in the IndexTable contained in the configuration file instead of both. Moreover, in the "Selector" column shown in figure 2.13, one selects which items within that aspect (for example, SSP2) will be used.

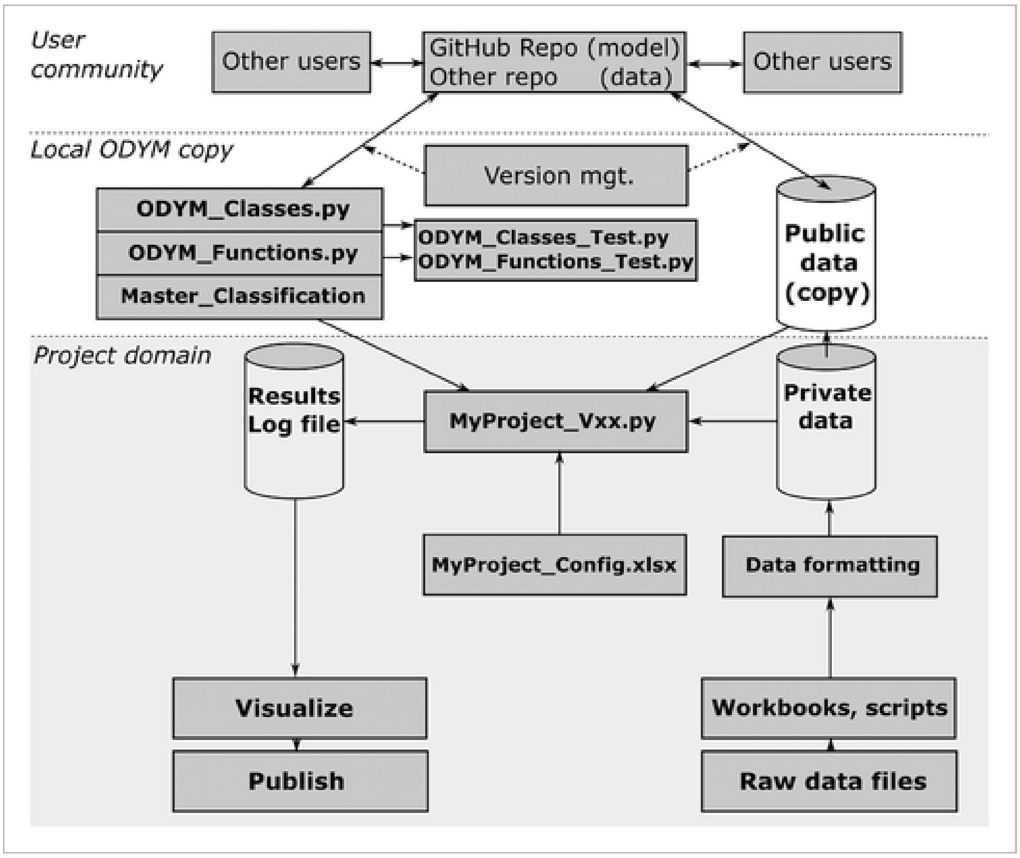


Figure 2.17: Structure of ODYM domains (Source: PAULIUK and HEEREN (2020b))

The project database may come from a combination of data from other projects along with data specifically acquired for the current project. The next section will briefly address how version 2.5 of the RECC incorporated new data into version 2.4 for the analysis of new consumption sectors. For this purpose, it was necessary to modify the configuration spreadsheet, but not necessarily the Classification_Master sheet. If the latter was designed anticipating future changes, the list of aspects may already include new implementations. However, the database and the list of parameters will need to be updated.

The database is contained in other spreadsheets, each referenced by the name of the corresponding parameter. This strategy, along with the use of multidimensional vectors, allows for ease in analyzing different scenarios. For example, an analysis of material efficiency can be done by increasing the lifespan of consumer goods. For this case, simply change the data in one column of a table; or insert a new column with data whose header is the name of the new scenario; or, as a last alternative, use a multiplier, whose input comes from another file in the database, which can be properly operated through the `einsum` on the vector that one wishes to alter.

ID	Name	Symbol	Description
1	**Flow**		**Objects flowing between processes**
	Flow	F	
2	**Stock**		**Objects residing as stocks in processes**
	Stock	S	General stock
	In-use stock	IUS	
	Population	P	
3	**Material/Product property**		**Intensive object properties**
	Lifetime	LT	
	Material composition	MC	
	Share	SHA	
	Intensity of use	IU	
	Specific energy consumption	EI	
4	**Process coefficient (intensive)**		**Intensive process properties**
	Yield coefficient	PY	
	Process extension	PE	
	Process factor (per capacity)	PF	
5	**Extensive process property**		**Extensive process properties such as capacity**
	Process capacity	CAP	
6	**General Ratio**		
	Per capita stock/flow	PCS PCF	Any ratio between two system variables from the groups 1-5 above
7	**Correspondence table**	CT	Correspondence between two classifications
8	**General**	FLAG	Boolean value (to flag a certain property)

Figure 2.18: Structure of the database nomenclature (Source: PAULIUK (2023))

The database can contain parameters in three broad categories, which are: socioeconomic such as population, GDP, average vehicle occupancy, and inhabitants per dwelling; technological such as equipment lifespan, efficiency rates, material intensity, among a multitude of others; and finally, material efficiency parameters, which typically are modifications to parameters in one of the previous two categories, such as a multiplier for increasing car usage in a carsharing scenario enabled by technology or regulation. ODYM also proposes a way of naming this database and a method of recording each data set aimed at maintaining historical and traceability. The table in figure 2.18 shows the nomenclature used in each parameter group. Meanwhile, figure 2.19 shows the first page of each data set in the database, in this case, the material composition of passenger vehicles. This page contains metadata such as source, description, scope, year, and date of access.

This construction method allows for the collaborative development of a more

DATASET

Item	Description	Example
Dataset Name	Serves as description	*Material composition of passenger vehicles, extracted from Hawkins et al. (2013) inventory.*
Dataset version	if any	*none*
Type of data	E.g., stock, flow, lifetime, product (	*product material composition*
Process scope	if any	*none*
Process resolution	if any	*none*
Product scope	if any	*passenger vehicles*
Product resolution	if any	*ICE vehicle, battery electric vehicle, fuel cell vehicle*
Material scope	if any	*metals, polymers, silica material, chemicals, other*
Material resolution	if any	*42 materials*
Regional scope	if any	*global*
Regional resolution	if any	*global*
Temporal scope	if any	*ca. 2000-2010*
Temporal resolution	if any	*ca. 2000-2010*
Semantic string example	"The copper content of average typ	*"The zinc content of average ICE vehicles, ca. 2000-2010 vintage, is 0.0998 kg / unit."*
Keywords	3-5 descriptive keywords	*product material composition; metal content; passenger vehicles*
Data provenance	Expert estimates, mass balance, pı	*industry data*
Type of source	publicly available dataset or report	*supplementary material of journal article*
Dataset format	Select 1 of the following:	*Excel spreadsheet*
Dataset license	if any	*CC-BY*
Main/first author or organisation		*Troy R. Hawkins*
Link to dataset	if any	*https://onlinelibrary.wiley.com/action/downloadSupplement?doi=10.1111%2Fj.1530-9290.2012.00532.x&attc*
Link to accompanying report/paper	if any	*https://onlinelibrary.wiley.com/doi/abs/10.1111/j.1530-9290.2012.00532.x*
Suggested citation	DOI sufficient	*10.1111/j.1530-9290.2012.00532.x*
Access date	Data on which data were accessed	*04.06.2018*
Entry author	Your name	*Stefan Pauliuk*

Data/Unit/Uncertainty/Comment as tables or list

Up to you how to organise this best!

Material	Unit	Vehicle type internal combustion engine	Vehicle type battery electric vehicle	Vehicle type fuel cell vehicle	Uncertainty
steel	kg/unit	882.0902775	923.3628638	1158.098555	None
iron	kg/unit	115.8742446	20.81181057	20.81181057	None
aluminium	kg/unit	71.2499941	111.8435601	80.6365339	None
copper	kg/unit	23.87236603	67.53263096	38.91757181	None
magnesium	kg/unit	0.240403956	0.240403956	0.240403956	None
zinc	kg/unit	0.099790321	0.099790321	0.099790321	None

Figure 2.19: Structure of the a dataset metadata (Source: PAULIUK (2023))

robust model. New features can be added with each academic work, such as a technological route, a new material, etc., scaling the model's scope step by step. Figure 2.20 illustrates the development roadmap of the IE group at the University of Freiburg.

Once the MFA system is defined, model equations must be programmed in the Python script, adhering to the mass balance principle. The ODYM includes a special library for dynamic MFA, defined in dynamic_stock_model.py, which can handle various stock-flow relations in dynamic stock modeling, including inflow-driven and stock-driven models.

Modeling the equations is not trivial and is closely linked to the structure of the proposed model (its processes, flows, scope, issues to investigate, etc.) and the database. However, there is some flexibility in changing the values used in the database by making the necessary changes in the code, as well as proposing another modeling approach and making use of the database. As will be discussed later, the RECC, built on the ODYM platform, offers a solid model with consolidated data that could be adapted to work with data from another IAM, skipping the costly stages of modeling from scratch.

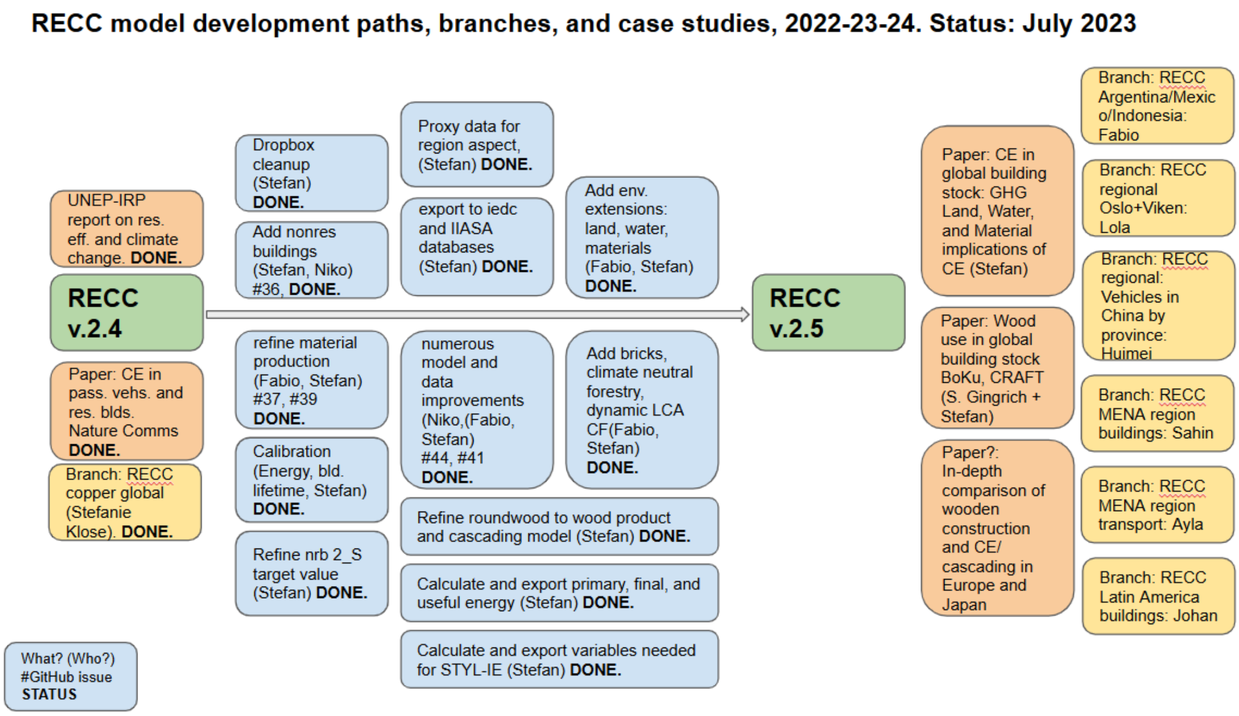


Figure 2.20: RECC's developing roadmap

2.4.2 RECC

2.4.2.1 Research Questions

This section is based on the documentation of the RECC model (PAULIUK, 2023). The RECC is a project that encompasses a dMFA model built within the ODYM framework aimed at answering the following questions:

1. What is the impact of the different material efficiency strategies on material cycles, energy use, GHG emissions, and raw material extraction for different socioeconomic scenarios until 2060?

2. How large are the trade-offs and co-benefits of the different material efficiency strategies when implemented together?

3. How do socioeconomic or lifestyle changes translate into lower material use and what are the possible GHG and raw material savings until 2060?

4. How big is the impact of material efficiency strategies on burden shifting across sectors and on the life cycle performance indicators of products and services?

2.4.2.2 Model Characterization

The project was set up with the structure shown in figure 2.21. It is possible to identify that the dMFA model is fed with three groups of data and assumptions:

those from the socioeconomic narratives, the sector modeling responsible for describing the service demand, and data that integrate the model into the LCI analysis. The description of the processes, flows, and ME strategies can be seen in figure 2.22.

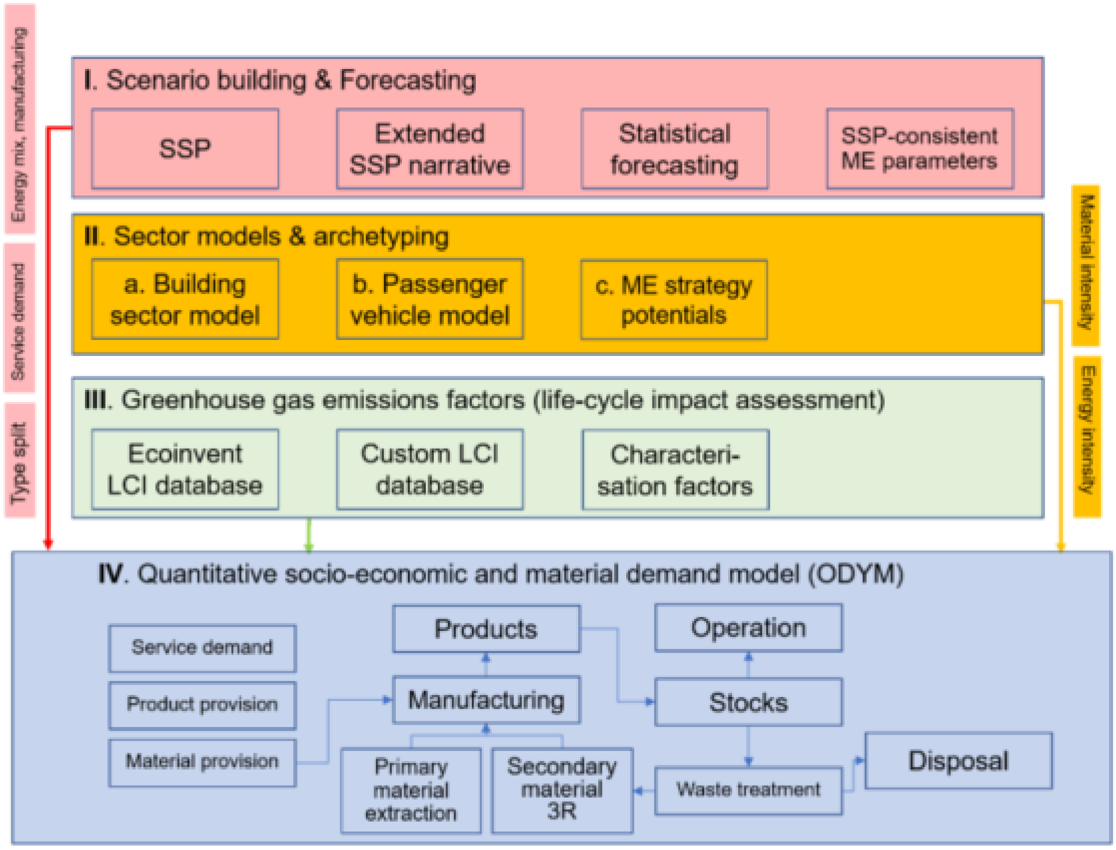


Figure 2.21: RECC's project structure (Source: (PAULIUK, 2023))

From the definitions of the MFA, the RECC can be defined by:

Time scope: The total time frame is from 1900-2060. This period is divided between the modeled period (future projection) from 2016 to 2060 and before 2016, years in which historical data are used to estimate current stocks and calibrate the system.

Engineering materials: The following engineering materials are evaluated in the RECC: construction grade steel, automotive steel, stainless steel, cast iron, wrought Al, cast Al, copper electric grade, plastics, cement, wood and wood products, zinc, concrete, concrete aggregates, bricks, glass, insulation material.

Products: Passenger vehicles are divided into 6 technology types: Internal Combustion Engine, gasoline (ICEG), Internal Combustion Engine, diesel (ICED), Hybrid Electric Vehicles (HEV), Plugin Hybrid Electric Vehicles (PHEV), Battery Electric Vehicles (BEV), Fuel Cell Vehicles (FCV) and into 4 segments: microcar, passenger car, minivan_SUV, and light truck.

There are 12 types of residential buildings addressed divided into SFH, MFH,

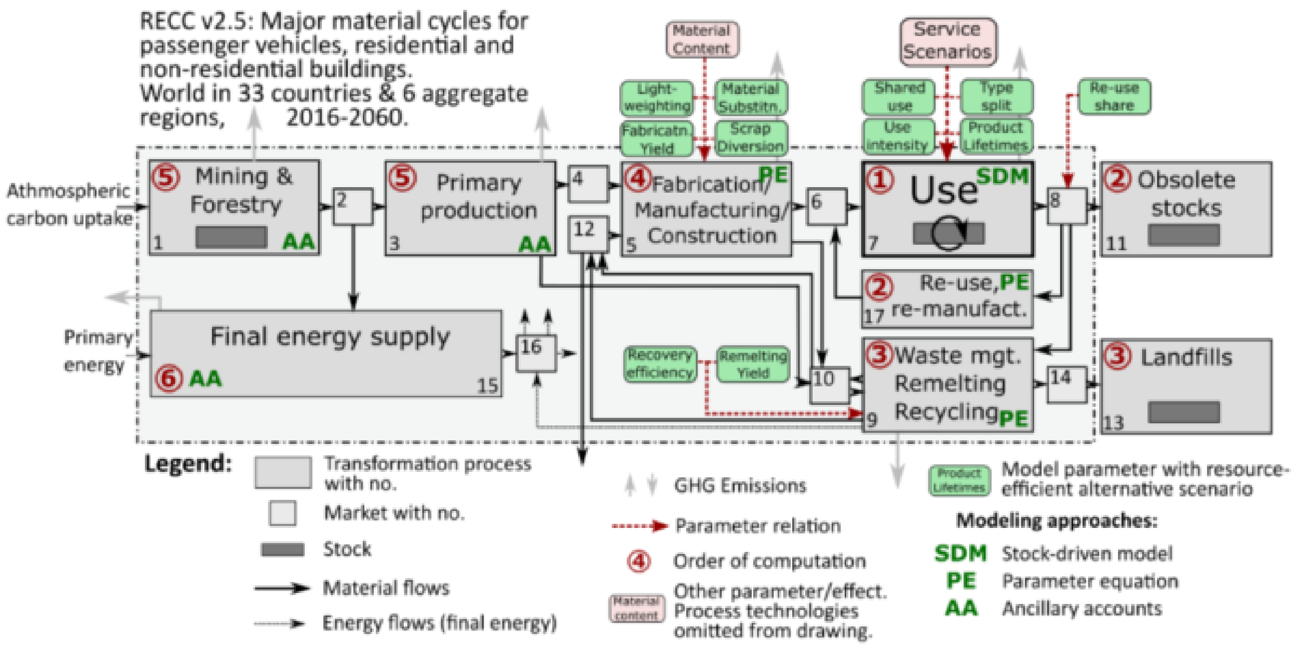


Figure 2.22: RECC's dMFA structure (Source: (PAULIUK, 2023))

and RT each of which can be non-standard, standard, efficient, and ZEB, where SFH is a single-family house, MFH is a multi-family house, RT is a residential tower, and ZEB stands for Zero Energy Building. The types of non-residential buildings are 24, which can be offices, commercial, educational, health, hotels & restaurants, and others; each of these also has one of the 4 categorizations used in residential.

Appliances include 12 types: Fan, Air-cooler, Air-conditioning, Refrigerator, Microwave, Washing Machine, Tumble dryer, Dishwasher, Television, VCR/DVD player, PC & Laptop computers, Other small appliances.

There are 18 technologies for electric power generation included: solar photovoltaic power plant, concentrating solar power plant (CSP), wind power plant onshore, wind power plant offshore, hydro power plant, nuclear power plant, coal power plant, coal power plant without abatement measures, bio power plant, oil power plant, geothermal power plant, IGCC power plant, light oil combined cycle, gas combined cycle power plant, advanced coal power plant with CCS, coal power plant with CCS, biomass power plant with CCS, gas combined cycle power plant with CCS.

Finally, there is a plan to model road and rail infrastructures in the future.

Scenarios: Six scenarios are used, given by the combination of three socioeconomic scenarios: LED (low energy demand), SSP1, SSP2, and two climate policy scenarios: RCP2.6, and a baseline scenario, where no new climate policy is adopted after 2020. In the declaration of aspects, the socioeconomic scenarios are given by `SSP_scenarios` and the climate policy scenarios by `RCP_scenarios`

Energy carriers: The following energy carriers are described: Electricity, Coal, Hard Coal, Diesel, Gasoline, Natural Gas, Hydrogen, and Fuel Wood.

Environmental Impacts: The following environmental impacts & demands are either implemented or planned to be implemented: GWP100, Land Occupation (LOP), Water Consumption Potential (WCP), Fossil Fuels Raw Material Input RMI, Metal Ores RMI, Non-metallic Minerals RMI, Biomass RMI, Abiotic Materials RMI, Primary Energy Demand.

Emissions: Emissions of the same three GHGs as in COFFEE are assessed: CO_2, CH_4, and nitrous oxide N_2O

Chemical Elements: C, Al, Cr, Fe, Cu, Zn, 'Other'

Process: There is a material production process for each "material production" technology; a manufacturing and a use phase process for each final product. Finally, there is a waste management process "to convert each of the 15 products into waste/scrap at the end of life, one remelting process for each scrap category" (PAULIUK, 2023).

Waste process: A single waste management process (including dismantling, shredding, and sorting) is used to convert each of the 15 products into waste or scrap at the end of their life cycle, followed by a remelting process for each scrap category

Regions: The regional resolution varies and can be described in 32 regions, 11 regions, 5 regions, or as a global region. This depends on the focus of the model run and, above all, on data availability or applicability based on the structure of ODYM. Factors such as the lifespan of goods and equipment, when declared within the model, may exhibit regional differences and explicitly include this aspect. However, in cases such as the lifespan of a hydroelectric plant, for example, a single global factor tends to be applied. Although regional differences may exist, the modelers determined that differentiation across regions would not be relevant in such cases, so a single-region resolution is used. The regions division is based on SSP Database version 2.0 available at `https://tntcat.iiasa.ac.at/SspDb/dsd?Action=htmlpage&page=about` and is shown in table 2.7

2.4.2.3 RECC Strategies

The RECC model operates with the following ME strategies:

- End-of-life recovery rate improvement (**EoL**)
- Fabrication yield improvement (**FYI**)
- Fabrication scrap diversion (**FSD**)
- Reuse (**ReU**)
- Lifetime extension (**LTE**)
- Material substitution (**MSU**)

Table 2.7: Regional Classifications in ODYM-RECC

32 regions			11 regions	5 regions
R32AUNZ	R32IDN	R32OAS-L	AFR	R5.OECD
R32BRA	R32IND	R32OAS-M	CPA	R5.2REF
R32CAN	R32JPN	R32PAK	EEU	R5.2MAF
R32CAS	R32KOR	R32RUS	FSU	R5.2LAM
R32CHN	R32LAM-L	R32SAF	LAC	R5.2ASIA
R32EEU	R32LAM-M	R32SSA-L	MEA	
R32EEU-FSU	R32MEA-H	R32SSA-M	NAM	
R32EFTA	R32MEA-M	R32TUR	PAO	
R32EU12-H	R32MEX	R32TWN	PAS	
R32EU12-M	R32NAF	R32USA	SAS	
R32EU15	R32OAS-CPA		WEU	

- Using less material by design / down-sizing (**ULD**)
- Car-sharing * (**CaS**)
- Ride-sharing for cars * (**RiS**)
- More intensive use of floor space # (**MIU**)

As Figure 2.22 suggests, these strategies can operate at different phases of the material cycle and are implemented in a cascading manner. For a detailed description of their implementation (start year, reduction factors, etc.), see PAULIUK (2023)[p.41].

It is important to note that, in an integration process with an IAM, some ME strategies may be omitted or not implemented by ODYM-RECC to avoid duplicating efficiency scenarios. For example, an IAM may already include a scenario for adopting a lighter vehicle fleet or migrating to public transport. In such cases, the vehicle fleet demand and its typology would be provided by the IAM.

2.4.2.4 ODYM-RECC's Inputs and Outputs

Part of this study will involve a detailed diagnosis of the inputs and outputs of ODYM. However, at a broader level, and based on the literature already produced with it, a brief description of both can be made. Versions 2.4 and 2.5 of the model were responsible for producing materials such as the following technical reports: (IRP *et al.*, 2020), (JAKTAR *et al.*, 2024b), (JAKTAR *et al.*, 2024c), (JAKTAR *et al.*, 2024a), and (HERTWICH *et al.*, 2019a); and the following scientific articles: (VÉLEZ-HENAO and PAULIUK, 2024), (PAULIUK *et al.*, 2024), (PAULIUK *et al.*, 2021d), (FISHMAN *et al.*, 2021a), (KLOSE and PAULIUK, 2023), (PAULIUK and HEEREN, 2020a), and (PAULIUK *et al.*, 2021a), which are compiled on the Zenodo platform in (HERTWICH *et al.*, 2020).

To create an interrelationship with the IAM framework, macroeconomic data from SSP1, SSP2, and LED scenarios, available in the IIASA database, are typically used. For some publications, data on transport services in tkm and pkm, as well as housing and built area services, are taken from IAM runs such as IMAGE and MESSAGE. Inputs are provided in the form of Excel tables read by the ODYM-RECC script and will be discussed in detail later. Basic data required to run the system include parameters for the lifespan of evaluated consumer products (type of statistical distribution and its parameters); stock of these products at the simulation start year; average lifespan of stocks in use; material intensities for manufacturing final goods or engineering materials; production yields (losses, efficiency, etc.); distribution of goods by archetype type and trends in their share over time; recycling rates of discarded goods and reuse yields; and environmental impacts such as CO_2 emitted per item/mass produced.

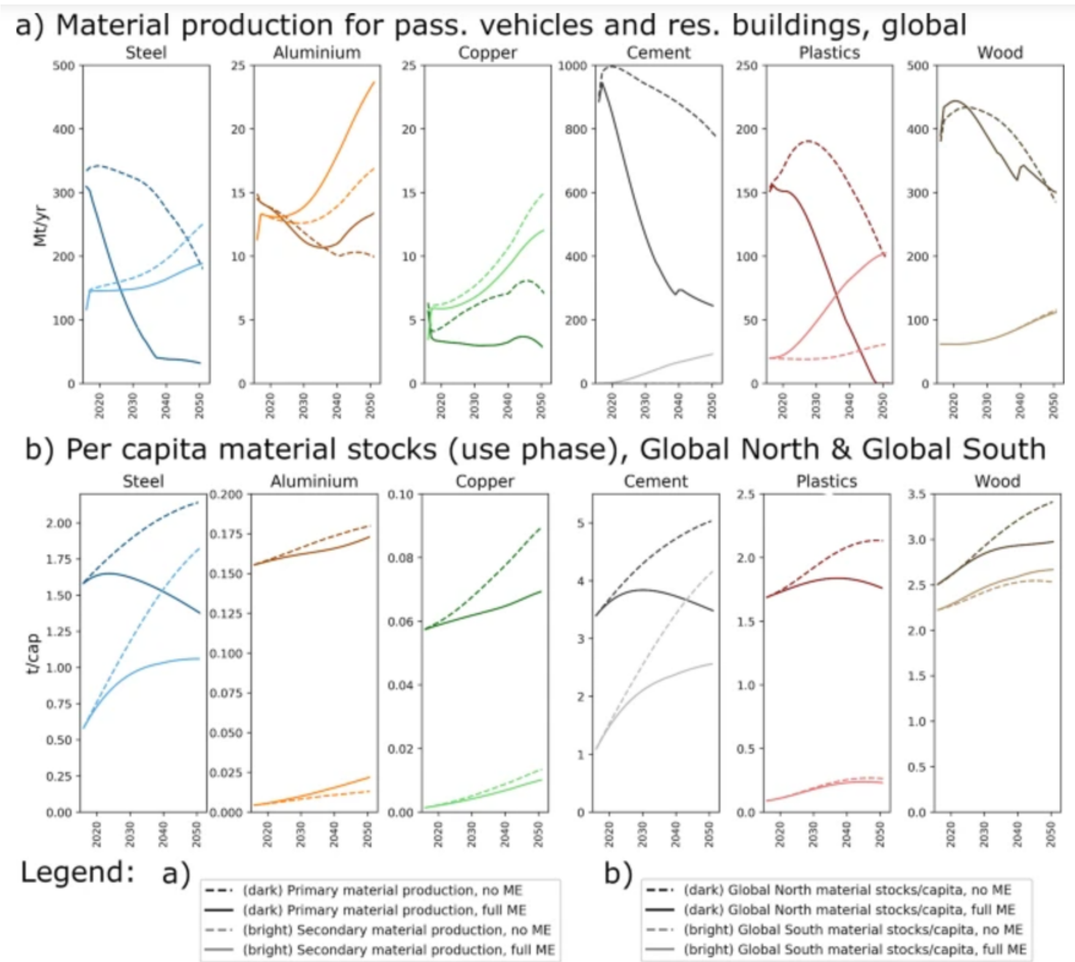


Figure 2.23: And example of ODYM-RECC's output (Source: (PAULIUK *et al.*, 2021d))

The primary outputs are material stocks and flows (inflows and outflows) across various phases (production, use, etc.) evaluated in the model. Furthermore, with a focus on emissions, nearly all of the scientific materials listed above calculate

GHG emissions from the evaluated sectors. In the latest version, 2.5, some other environmental impacts can also be assessed, such as potential water consumption, SF6 emissions, among others. For the scope of this study, the demand for primary materials is probably the most relevant output. In this regard, it is worth illustrating examples of this output from previously produced material, as shown in Figure 2.23.

2.4.3 Gaps in IAMs Potentially Addressed by Dynamic MFA using ODYM

2.4.3.1 Transparency and Cooperation

The previous section introduced the general structure of the ODYM RECC model. It's important to note that its construction was possible due to certain aspects that already differ from those in the development of IAMs, and which constitute part of the criticism against them. The first is complete transparency: the code is open-source, available on the GitHub platform, and written in Python, which is widely used globally. The platform allows for change control, branching, and forum discussion. The use of the software is facilitated by updated documentation (PAULIUK, 2023), (PAULIUK and HEEREN, 2020b), (PAULIUK *et al.*, 2021a), and courses with usage examples (INDUSTRIAL ECOLOGY FREIBURG, 2018). From the standpoint of input data, there is also great transparency, with data located on a public platform (INDUSTRIAL ECOLOGY FREIBURG, 2024a); each database file explicitly cites the data source as well as any assumptions involved in its manipulation.

Moreover, in the integration process between IAMs and the ODYM-RECC model, there will be a need to open up internal IAM data that must be harmonized with ODYM. Examples could include assumptions about inhabitants per residence or process emissions considered per mass of cement. In (PAULIUK *et al.*, 2021d), the raw database used is provided on the Zenodo platform in (PAULIUK *et al.*, 2021b) and the results in (PAULIUK *et al.*, 2021c). The same methodology could be adopted to maintain and add to the philosophy of transparency.

The second aspect is the creation of an open and cooperative environment, easied by transparency. The software is licensed under the MIT License, which permits commercial use, modifications, distribution, and private use, but does not include liability or warranty (OPEN SOURCE INITIATIVE, N/A). Creating branches in the software via GitHub or in private environments allows different research groups to adapt the program to their specific needs. The data platform was also built in a structured, open, and participative way. This type of environment creates a common work framework that allows for future result comparisons and the proposition of common critiques for improvement.

The advantages presented above represent an overcoming of the IAM development paradigm, which occurred on different platforms with various degrees of transparency in assumptions and input data. Clearly, dMFA is a method, and building a platform for its integrated use with IAMs tends to be less complex than building an IAM itself. However, given the proposal to cover an existing gap, ODYM-RECC starts from a point that already avoids certain criticisms of IAMs.

In addition to the philosophy of construction, other potential aspects of the integration between the ODYM-RECC dMFA model and IAMs will be analyzed.

2.4.3.2 Representation of Material Cycles and Link Between Stocks and Services

As discussed in section 2.1.3, there is a lack of a link between material stocks and the services provided. Some studies have already made this link through the use of inputs and/or outputs from IAMs as inputs to ODYM (KLOSE and PAULIUK, 2023), (DEETMAN *et al.*, 2021), (PAULIUK *et al.*, 2021d). An example of this link can be seen in the transportation sector. An IAM might take as input a certain amount of services offered, such as passenger-kilometers, which will be met by the energy system with a pool of energy sources. However, in many IAMs, there is no link with the stock of vehicles necessary to meet this demand, which is a common case when the service input in the partial equilibrium model is provided by the CGE. In the case of COFFEE, this link exists; the ICCT model provides the quantity of vehicles distributed by type and technology, however, there is a lack of a link between demanded the vehicles stocks and stocks and flows of materials demanded. For example, a decarbonization scenario that requires a higher demand for electric vehicles will also require more materials such as copper and lithium, and this is not evaluated within the IAM.

This leads to a second point, which is the better evaluation of material cycles. As seen in figure 2.6, this cycle goes through various stages that can be evaluated in detail. At each stage, there are losses, energy use, potential demand for natural resources such as water, GHG emissions, etc. that can be assessed through the integration of dMFA and Life Cycle Assessment (LCA) methods. This integration is proposed, for example, by (PAULIUK *et al.*, 2017) and (GAMBHIR *et al.*, 2019). By using LCA inventory data, it's possible to link the quantity of material produced to these impacts, depending on the production route of the material, the origin of the raw materials, and the processing, among other characteristics. Any scenario run on an IAM that does not consider the impact that an increased demand for materials will have on the biosphere will result in an incomplete assessment of the real limits of that scenario. Thus, thoroughly tracing the cycle of a material can indicate externalities not identified within an IAM. It can also highlight potential gains with material efficiency (ME), process optimization, increased collection for recycling, among others. Pauliuk et al (PAULIUK *et al.*, 2021d) evaluate how ME strategies can contribute to emission reductions. The IEA has a schematic model of some ME strategies that can be applied in each cycle as shown in figure 2.24.

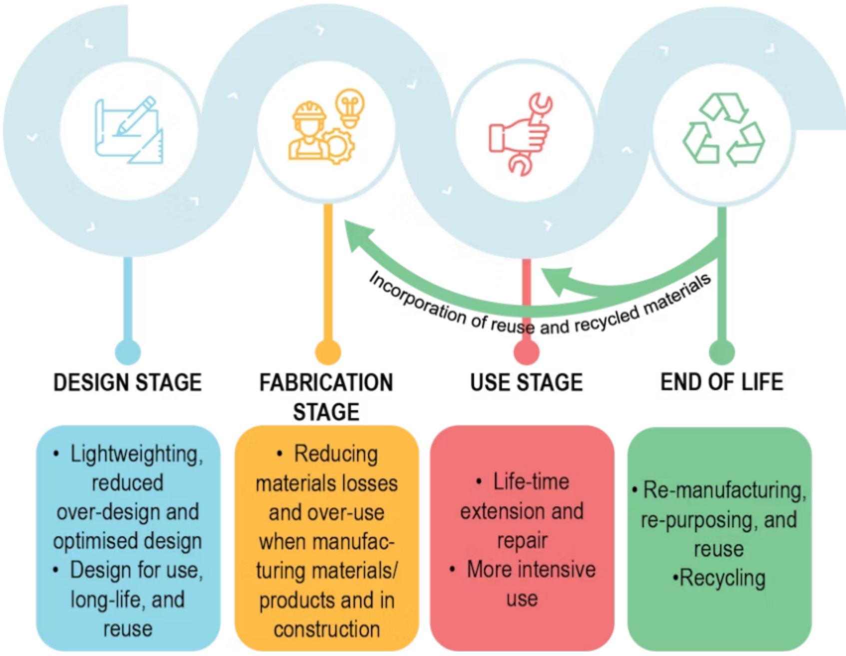


Figure 2.24: Material efficiency strategies applicable to each stage in material cycles. (Source: (IEA, 2019))

2.4.3.3 Feasibility

Another possible evaluation using dMFA is feasibility assessment. The previously described increase in demand may encounter issues with insufficient stocks and flows. A model like ODYM allows for the insertion of estimated reserves and the evaluation of a material's primary production. If the demand for a material approaches its estimated reserves, for example, this indicates a potential restriction on the scenario in question.

Regarding flow issues, sudden spikes in demand occurring over short periods can indicate a temporary restriction of a material, which could limit the realization of the projected scenario or cause delays. This is because, in some sectors such as mining, the time to implement new projects can be long and may not match the dynamics of demand. dMFA models can identify such constraints. So, a soft-link can provide a supply constraint of a particular service on an IAM, or on stocks such as vehicle ones in the COFFEE model.

Feasibility analysis can also be conducted from the perspective of constraints on the socio-environmental damages caused in the material cycle (BAARS *et al.*, 2022). Copper, for example, has its reserves concentrated in areas of critical water scarcity

(NORTHEY *et al.*, 2019), and a spike in its demand could lead to significant social impacts. Again, a water constraint imposed can feed back into the IAM via a service or maximum stock constraint.

2.4.3.4 Improve feedbacks to IAMs and CGEs

dMFA models do not internally evaluate material costs, however, they can provide information for economic models that do (BAARS *et al.*, 2022). The specific demand constraints described previously could lead to a surge in prices. Modeling through demand elasticity curves that receive inputs from dMFA could be an alternative. Evaluating prices by incorporating environmental costs (carbon pricing, water and land use) could be another alternative. Moreover, the increase in the cost of primary materials can feedback into the costs of the technologies implemented.

A second feedback that dMFA models could provide is about stocks still in operation. As discussed earlier, the lifespan of assets in IAMs is typically fixed, with each having a certain number of years of operation after which it is discontinued and needs to be replaced. dMFAs have the characteristic of better estimating the discontinuation rate of assets using probability distributions compiled in the literature. Thus, the IAM would provide the dMFA with the type of asset and the year it enters operation, while the dMFA would feed back to the IAM the year that the asset is discontinued.

A third possible feedback involves data on energy. As detailed in the sections describing ODYM and in the "spatial resolution" subsection, defining the system in multiple aspects and using the Einsum tool facilitate this analysis. For example, one could link the energy intensity in the production of a particular consumer good (aspect "Goods" and index letter g), which utilized certain engineering materials (aspect "Engineering materials" with index letter m), manufactured through their respective processes (aspect "MaterialProductionProcesse" and index letter P) in a specific region (aspect "Region" and different index letters depending on the aggregation). The total calculated energy consumption can provide feedback for a better evaluation of energy demand, conducted in a more disaggregated and bottom-up method, particularly for sectors that are more energy-intensive and/or more impacted by transition scenarios.

Finally, another possible feedback could be the consistency analysis of certain material evaluations conducted within an IAM. In industrial sectors where there is already a projection of demand (usually cement, steel, and petrochemicals), a consistency analysis can be performed to check if that input generates a stock adequate to meet the service demand given by the IAM itself or by its associated CGE.

Given the above, the following chapter proposes a methodology for a comprehensive diagnosis of the models discussed above in order to propose their integration.

3 Methodology

3.1 Diagnose of COFFEE structure, resolution, inputs and outputs

As previously described, the objective of this study is to propose a methodology for integration via soft-link between COFFEE-TEA and ODYM-RECC. For this, it is essential to understand which outputs from the former can be used to inform the latter, and vice versa. Another key adjustment is the alignment of specific parameters, such as time steps and regions.

The definition of the structure is crucial for understanding the data flow. Part of this structure was described in the previous chapter. Throughout a given run, a piece of data has an origin, may be transformed into something else, and/or may serve as input for part of the model. Understanding this flow, the origin of the data (whether generated endogenously or exogenously), where in the model it is generated, and what it informs is essential for integration. Alternatives for inputs should also be considered. COFFEE can be integrated with TEA or receive macroeconomic data from pre-established scenarios, including those from IAM consortia. In the latter case, for example, sectoral demands do not necessarily undergo a macroeconomic consistency analysis. If ODYM-RECC requires the same macroeconomic inputs, integration becomes simpler as there is no need for a soft-link between it and the CGE model.

Understanding the model's resolution is also crucial for any integration. In the previous chapter, the COFFEE and TEA models and their soft-link integration were discussed. Regarding sectoral resolution, for instance, it becomes evident that not all sectors and subsectors described in COFFEE are disaggregated in the same way in TEA. The transport sector is one such case: while COFFEE distinguishes between passenger and freight transport, TEA differentiates between land, maritime, and air transport. This type of divergence in sectoral division and resolution necessitates adjustments in the interface between the models, which can be addressed either by making internal changes to the models to ensure compatibility or by externally processing the data to transform an output from one model into an input for the other.

As discussed above, IAMs do not always provide clear or adequate documentation of these parameters. In some cases, their structure, level of detail, internal loops, and other aspects are not properly organized in a manual or any other type of documentation. In this regard, PAULIUK *et al.* (2017) proposes a diagnostic methodology for IAMs to assist in this understanding. The methodology is compiled in two spreadsheets, each containing a series of questions. The first, with 93 questions, addresses the model's structure, while the second, with 51 questions, focuses on its resolution. The first set of questions explores the inputs and outputs, internal loops, covered sectors, the mathematical model, how energy demands are calculated, among other elements. The second set of questions deals with the model's resolution, covering the number of regions, generation technologies, types of transport modes, etc. These tables will be reproduced in the results chapter, along with the corresponding answers for COFFEE-TEA. During the response collection process, it was deemed necessary to add a question on the chemical industry and another on the metals industry (excluding iron and steel) to the structure section.

Part of this description has already been provided in the previous chapter - although not formalized within the specified framework - using the available documentation for COFFEE and TEA. Since not all documentation has been updated following the IAM updates, as noted in PAULIUK *et al.* (2017), some data acquisition will be carried out through direct contact with the current COFFEE modelers at the Centre for Energy and Environmental Economic (CENERGIA). Another important source of data for tracking model changes will come from doctoral theses and master's dissertations that, within their scopes, have modified and enhanced the COFFEE model.

3.2 Diagnose of ODYM-RECC structure, resolution, inputs and outputs

For ODYM, the model's structure and resolution are extensively described in its documentation. Its inputs are primarily defined by the database. Section 5.2 and 5.4 in PAULIUK (2023) provides the full list of parameters and input data used in the model, including resolution, which is generally defined by the aspects of ODYM described in section 2.4.1.1. The data resolutions to be used in ODYM-RECC and COFFEE-TEA that differ, such as the vehicle fleet, must necessarily be harmonized.

These parameters are divided into socioeconomic, technological, and resource efficiency categories. In the first class of parameters are those such as population growth, which are also used in COFFEE. Others, like building stocks, vehicle stocks, future demand for appliances, and product lifetimes, are not necessarily required by the IAM. In the second class, there are data such as material intensities of final products, recycling yields, scrap recovery efficiencies, among others. It is important to note that a considerable amount of data has been collected, which saves time during integration and avoids laborious data gathering. Some of this data, such as vehicle conversion efficiency or energy demand per square meter of residential area, is necessarily used in COFFEE and will require harmonization. Finally, the third class of parameters refers to changes in various other parameters intended for studying how they affect material demand. Examples include higher vehicle occupancy rates or lower energy demand per square meter of constructed area.

The following section will discuss a formal method for mapping what type of adjustment or harmonization each parameter will need for integration between the two models.

As said, the inputs are well described, on the other hand, the outputs are not as clearly defined in the documentation and largely depend on the RECC scenario used, both in terms of which outputs are generated and how their values vary. Diagnosing these outputs will require a combination of the official documentation, an interpretation of the program's code, and the analysis of results given in the Zenodo database (PAULIUK, 2024).

Essentially, the outputs can be divided into: environmental impacts, subdivided into atmospheric GHG emissions, potential water consumption, and land use; energy consumption; inflows over time, subdivided into finished products, engineering materials, and primary materials; outflows over time, also subdivided in the same manner as the inflows; and stock formation. Each of these outputs can also be segregated into the use and production phases, and occasionally into production goods (e.g., inflow of engineering materials for the production phase of light hybrid cars).

3.2.1 AI use in interpreting code

Another approach used for analyzing the ODYM-RECC code was training a chat within ChatGPT 4o. This tool allows for the insertion of instructions and materials for its training and serves as a database for consultation. Figure 3.1 shows the page for inserting instructions and materials, and in Appendix I, the instructions and files provided can be consulted. There will be no discussion here of artificial intelligence models or debates about the reliability of their use. All outputs provided by the trained chat were carefully verified against the ODYM-RECC code, scientific literature, or critically analyzed by the author of this work; the tool was employed as a facilitator for identifying code structures, interpreting their functions and provide insights on the integration between COFFEE and ODYM-RECC.

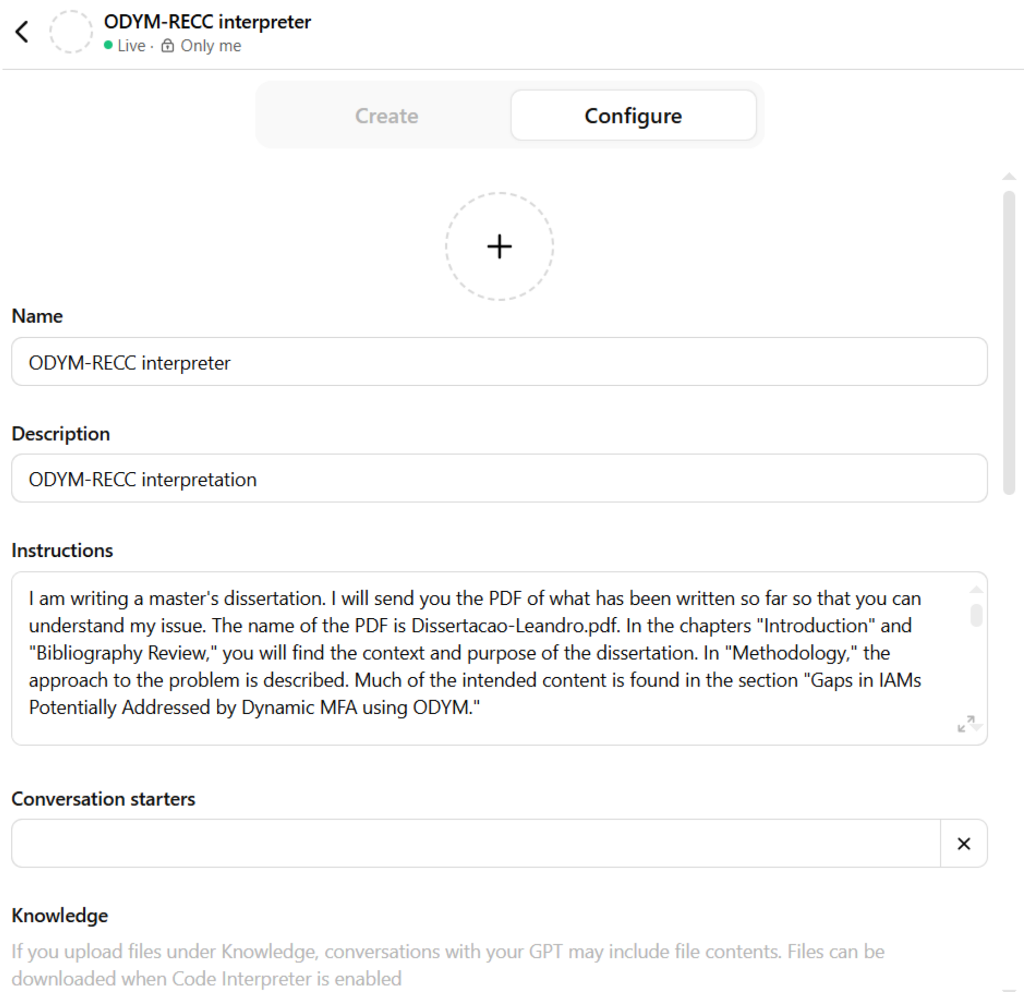


Figure 3.1: Screenshot of the setup page for creating a new chat in ChatGPT 4o

3.2.2 ODYM-RECC's Code Interpretation

Understanding the inputs and outputs of ODYM-RECC also involves understanding how they are read, declared, stored, manipulated, and what final results are obtained. Therefore, it will be important to include snippets of interpreted code that assist in this diagnosis. For this purpose, the declaration of the dMFA system, the reading and declaration of processes, parameters, flows, and stocks will be addressed. An exhaustive interpretation of the code will not be conducted, but rather one focused on addressing the interfaces for integration, i.e., the system's inputs and outputs.

3.3 Integration between COFFEE and ODYM-RECC

The previous diagnostic allows for the identification of divergence points, necessary adaptations, and possible feedback loops. For instance, COFFEE and ODYM-RECC might need to use the same car occupancy rates to estimate transport service demand, or alternatively, replace the estimate made in ODYM-RECC with the one used in COFFEE. Another example is the lifespan of a generation asset. COFFEE uses fixed parameters, where once the asset reaches the end of its life, a new capacity must be installed. On the other hand, ODYM-RECC makes an estimation using probability density curves, and its outputs can be used to feed back into COFFEE by providing the amount of generation capacity discontinued during a time step.

3.3.1 Buildings and Passenger Transport Sector

ODYM-RECC currently has two major sectors described that are common to COFFEE: the buildings and passenger transport sectors. For these sectors, both COFFEE and ODYM-RECC have their own methodologies for linking the energy service demanded (pkm, lighting, heating, etc.) to parameters that serve as proxies for measurement, such as fleet size, number of passengers, square meters of built area, inhabitants per dwelling, among others. For them, an integration proposal will be made that involves:

- comparing the input methodologies and suggesting which one will be maintained by evaluating advantages and disadvantages;
- assessing which database files become unnecessary, which need to be modified to use the same data source, and which should be maintained;
- suggesting a feasible integration in light of the diagnosis of the different resolutions between the two models. For example, cars with ethanol engines are not described in ODYM-RECC, whereas they are in COFFEE. It will be discussed how to address this difference in each sector's resolution.
- which ME strategies might be lost or not implemented by ODYM-RECC. For example, an IAM may include transport efficiency options, such as car-sharing scenarios, so the reduction in fleet demand would come from the scenario provided by the IAM to ODYM.

3.3.2 Future Sectors in ODYM-RECC

Although not yet included, the developers of ODYM-RECC intend to model additional sectors, such as power generation, transmission and distribution infrastructure, appliances, and transport infrastructure, including roads and railways. Part of this has been modeled by KLOSE and PAULIUK (2023) in a study using ODYM-RECC to model the copper cycle utilizing output data from IMAGE; the database has already been compiled and will likely be used, some of the files are already included in the ODYM-RECC v2.5 database. Therefore, a brief analysis of this integration will also be conducted.

3.3.3 ODYM-RECC Inputs

The proposed method for organizing this identification will involve analyzing the compatibility of each of the 120 input parameters in the ODYM-RECC input table. For each parameter, the following points will be evaluated:

- Needs compatibility between CGE-IAM?
- Which Aspects?
- Compatibility Action Description
- Comments on the Actions
- Can an Output from COFFEE or TEA be used as an Input Substitute?

To facilitate the analysis, the table contains the description of each parameter, its units and its aspects according to ODYM structure, as explained in section 2.4.1.1.

The first question aims to determine whether a dataset is used in both models, such as vehicle occupancy rates. If the answer is positive, it will be understood that harmonization is required.

The second question depends on the first. In the example mentioned, if COFFEE (or the data processing performed before input into the IAM) uses different factors for each region, this will be one of the aspects to be harmonized and indicated in this column.

The third point will describe indicative actions that may vary depending on the dataset. For instance, using the factors for the 18 regions in COFFEE could be an indicative action in the previous example. A simplification might also be chosen, such as using factors for 5 regions that will be applied to COFFEE. It is worth noting that preference will be given to altering the existing ODYM database rather than modifying COFFEE's data.

The fourth aspect will provide any general comments deemed important but that do not fit into the previous points.

Finally, the fifth question tends to indicate potential future integration via soft-linking. Just as ODYM-RECC uses part of its input data from IMAGE, this analysis will assess which outputs from COFFEE can feed into the ODYM model.

3.3.4 Time Resolution

An obvious requirement for integration is the need to harmonize temporal and regional resolutions. Regarding the former, COFFEE provides results at 5-year or 10-year intervals, so every output from COFFEE that will feed into ODYM must be adjusted accordingly, that is in a one year step. One way to achieve this is through cubic spline interpolation, which is commonly used to construct smooth curves that pass through the original data points. Unlike simple polynomial interpolation, which seeks a single curve for the entire set of points, cubic spline interpolation generates a third-degree (or lower) polynomial for each interval between two given points (MCKINLEY and LEVINE, 1998). As mentioned, the resulting function passes through the original points. For example, the installed generation data for the year 2045 provided by COFFEE will be the same as the input used in ODYM. One of the advantages of this method is that it ensures the resulting curve has no discontinuities and that both the first and second derivatives are continuous, producing a smooth curve with minimal oscillation, a feature also guaranteed by not using higher-order polynomials. To facilitate this harmonization, a Python script is proposed to expedite this conversion and is available in the Appendix II

Finally, another script is also suggested for extracting the annualized data provided by ODYM-RECC into the COFFEE format, with intervals of 5 years up to 2050 and 10 years up to 2100. The script is easily editable for cases where COFFEE is intended to run with 5-year intervals throughout the entire time horizon, for example. To achieve this, it is sufficient to modify the `desired_years` vector. This script it is also available in the same Appendix

3.3.5 ODYM-RECC Outputs

For the analysis of ODYM-RECC outputs, the same methodology used for inputs will be applied, with the difference that the final question will be replaced with "Can it be used as input for COFFEE or TEA?"

3.3.6 Discussion on Possible Structures and Scopes

There is a challenge in determining which of the two models will evaluate materials whose production is already addressed in COFFEE, particularly for the industrial sectors modeled within it. As previously mentioned, the demand for these materials in COFFEE is modeled as a proxy of a macroeconomic result, using a top-down perspective that does not necessarily capture changes resulting from mitigation policies. This demand, through a description of possible industrial processes to meet it, generates an energy demand. Meanwhile, ODYM-RECC conducts a bottom-up assessment, using material intensity factors to evaluate material demand based on service demand translated into final goods, also given as a proxy for macroeconomic indicators.

There could be three types of integration: the first, simpler, where ODYM would only perform a form of post-processing, verifying feasibility when it comes to reserves and environmental impacts. This analysis could result in feedback, imposing restrictions on certain technologies, for example. However, it would not contribute to a more detailed understanding of demand profile changes resulting from mitigation policies.

The second, more comprehensive and complex, would require that material demand be well described by ODYM, meaning the bottom-up analysis must ensure that all drivers of demand are represented. For this, the modeling work done by the University of Freiburg's group for each sector is essential. Currently, other sectors are still not covered in ODYM-RECC, such as telecommunications, freight fleets for inland waterway, maritime, and road transport; and aviation transport, among others. It is understood that this option is not yet feasible due to the lack of data or a preference to handle some sectors within the IAM, such as those industrial sectors already described.

A third and more viable option is, in the case of sectors not fully described in ODYM-RECC, to split the demand into two parts: one for those sectors that are adequately described and a second, generic part that encompasses all others. For example, cement demand could be divided into cement for housing, cement for services, cement for energy infrastructure and cement for road infrastructure—sectors described in ODYM-RECC — and another part as ”other cement.” This would require gathering data on current demand by sector and their shares, as well as future share projections. The ”other” share would evolve based on economic projections (given, for example, by CES curves), while the demand for those sectors modeled in ODYM would evolve as an endogenous variable according to the model's bottom-up analysis. These material demands would then be converted into energy demands to be addressed by COFFEE. It is important to note that ODYM-RECC includes an assessment of the energy required for each material, meaning that COFFEE could directly receive a vector containing the energy demand to be met.

The advantages, disadvantages, and feasibility of each proposal will be discussed depending on the results found. Furthermore, an analysis will be conducted on which gaps identified in chapter 2 can be addressed by each approach.

3.3.7 Diagram of the Integration

As previously discussed, in addition to the two main models to be integrated, COFFEE and ODYM-RECC, there is also the TEA, the CGE model and the Transportation Model, which is used to provide the fleet data for passenger and freight transport in the road transport sector. Additionally, there are other data sources, such as standard macroeconomic scenarios that serve as inputs for the models. As a method for illustrating the data flows between the models, a diagram of their integration will be proposed. The will not only indicate the information flows but also the sectoral segregations of each model.

4 Results

4.1 Structured description of COFFEE

As discussed in the Methodology chapter, this first section provides a detailed assessment of the structure and resolution of COFFEE/TEA. Each section presents tables with the analysis for these two aspects, divided into the following divisions and sectors:

- General Model Setup
- Macroeconomic and Policy Model
- Energy Conversion
- Transportation Sector
- Infrastructure Sector
- Buildings Sector
- Recycling and Waste Management Industries
- Industries and Material Production
- Land Use Model and Natural Resources

4.1.1 Structure Details

4.1.1.1 General Model Setup

Table 4.1: General Model Setup

GENERAL SETUP MODEL	
Question	**Answer**
What is the mathematical problem type and which type of solver is used?	COFFEE is based on MESSAGE, it suits the development of bottom-up models and PE models, with perfect foresight, solved through Linear Programming (LP). The TEA model is formulated as mixed complementary problem (MCP) and is solved through Mathematical Programming System for General Equilibrium (MPSGE3) within GAMS using the PATH solver.[a,b]

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Table 4.1 – continued from previous page

GENERAL SETUP MODEL	
Question	**Answer**
Is decision making modelled based on constrained optimization, market equilibrium, or on simulation?	Optimization, perfect foresight for COFFEE, while TEA runs into a dynamically recursive market equilibrium model. Equilibrium is reached when the following conditions are achieved: normal (zero) economic profit, market clearance, and balance of payment equal to zero.[a,b]
What is the main objective function/output of the model?	Minimization of total system costs (COFFEE); maximizing the inter-temporal utility function of a single representative producer-consumer in each world region (TEA).[a,b,c]
Which programming language(s) is used?	The model runs on the MESSAGE platform, which essentially consists of a model code (a compiled matrix generator written in C) and the post-processor. TEA models run in GAMS, using PATH Solver.[a,d]
Which are the exogenous drivers?	TEA: The main exogenous variables include the rate of economic and population growth; the growth of the workforce; the total factor productivity (TFP); structural changes in demand; formation of new capital; availability of backstop technologies; energy efficiency and energy intensity. COFFEE uses the same macroeconomic indicators added to the energy services demand given by TEA or other exogenous scenario generator.[c,e]
How is technology learning modelled?	For TEA: "The model assumes that there are technological changes in energy demand, given a reduction in the amount of energy per unit of GDP as each region's GDP per capita increases. Reductions in energy use per unit of product over time are characterized by technological changes, currently represented by the parameter AEEI (Autonomus Energy Efficiency Improvement), which is exogenously assumed to grow at the standard rate of 1%a.a". For COFFEE:In general, exogenous. Learning curves can be exogenously applied and reflected in technology cost. Usually it follows the "more installed, less cost" logic. [b, c]
How is behavioural change modelled?	Behaviour change is implicit in demand projections. TEA adjusts makes some baseline adjustments in long-term demand when necessary. Usually, parameters of GDP per capita and demand curves, or GDP per capita and demand share curves are adjusted to reflect some long-term preferences changes.[c,e]
How is population and its age structure modelled?	Population projections are exogenous (input through the scenario generator) and influence future energy baseline demand.[b,c]
How is GDP modelled?	GDP projections are an exogenous input into both TEA and COFFEE models. GDP projections are usually given by standard scenarios, like the SSPs ones.[b,c]

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Table 4.1 – continued from previous page

GENERAL SETUP MODEL	
Question	**Answer**
How is the model calibrated?	In the baseline, Total-Factor Productivity (TFP) is endogenously targeted to meet the GDP. Thus, both labor and capital productivity are endogenously defined, assuming that the evolution of total factor productivity will reproduce GDP levels. Labor supply follows population growth rates, such as the trend provided by the SSPs scenarios, and the workforce is derived (exogenously) from the population growth.[c]
How many economic (input-output) sectors are in the model?	Each region is modelled with 5 sectors and respective subsectors (2 subsectors for agriculture, 5 for energy, 4 for industry, 3 for Transport and 2 for services) in the economic model. For COFFEE, there are 6 sectors: Energy, Industrial, Residential, Services, Agriculture and Waste Management. Splits are describe below. model.[b, c]
What feedback mechanisms and nonlinearities are considered/not considered?	COFFEE is MESSAGE-based, so it's a dynamic linear optimization model. The main feedback loop is established between the general equilibrium model (TEA) and the energy partial equilibrium model (COFFEE). The first model provides optimized final energy demand, while the second provides final energy demand and costs. Primary energy sources are stratified into classes of quality, resulting in non-linear availability vs. cost of extraction curves.[b,c]

[a]Source: IAMC (2020)
[b]Source: ROCHEDO (2016)
[c]Source: CUNHA *et al.* (2020)
[d]Source: HUPPMANN *et al.* (2019)
[e]Class notes from COFFEE lecture

4.1.1.2 Macroeconomic and Policy Model

Table 4.2: Macroeconomic and Policy Model

MACROECONOMIC AND POLICY MODEL	
Question	**Answer**
How is demand for energy services modelled?	Total energy service demand is obtained from the economic model (TEA) and/or ICCT (transport sector). The distribution between sectors and subsectors (except for transport) is obtained by optimization in the energy-land use model (COFFEE). In the integration between TEA and COFFEE, the substitution elasticity between the different energy inputs is set equal to zero so that there is no substitutability between factors. The power generation branch has fixed input proportions and the penetration of different technologies carriers is determined by the COFFEE model.[c, b]

Continued on next page

Table 4.2 – continued from previous page

MACROECONOMIC AND POLICY MODEL	
Question	**Answer**
How are economy and energy system affected by the policies modelled?	In general, policies (including GHG emission pricing, caps and trade, renewable energy portfolio standards and other) are implemented via constraints or cost coefficients (negative and positive) in the optimization problem. For some mitigation strategies applied, refer to Table 7 of the Annex III of the AR6.[a]
How is the coupling between monetary and biophysical aspects of the economy modelled?	Through the coupling of COFFEE with TEA. TEA provides part of the sectoral macroeconomic demands that must be met by COFFEE's energy sector. Some sectoral demands, such as those from industries described in COFFEE, go through an intermediate process, which involves the description of production routes covered in COFFEE and that must later be supplied by its energy sector. In the case of soft-linking runs, COFFEE's output can serve as an input for macroeconomic closure in TEA.[c]
How is final energy demand determined?	Both models rely on the same exogenous population and GDP projections (e.g., SSP2). After its first run, TEA key outputs on sectoral production and private consumption are processed by a demand generator and serve as key inputs to COFFEE – particularly, energy service demands.[c]
How are labour constraints considered?	Total labour and work-age population is determined from external scenarios. In the calibration, labour and capital productivity are endogenously determined in order to meet GDP projections given by the scenario.[c]
How is the available personal/household income coupled to energy demand?	Demand for goods and services grows as household income increases in the General Equilibrium Model (TEA), being energy included in "goods and services". Additional adjustments in long-term demand can be made based on estimated curves relating to GDP per capita and demand share.[c]
How does the age structure of the population affect labour supply and demand for goods, services, and energy?	There is no link between population age and changes in the demand for services, goods, and energy in COFFEE. For the macroeconomic model, the economically active population is provided exogenously, with a potential connection between population age and the workforce. Labor, as a factor of production, is related to the available workforce but depends on Total Factor Productivity, which is given endogenously to achieve the GDP supplied to the system.[b, c]
How does the available capacity/capital stock constrain output?	The capital stock is one of the production factors given as input in the general equilibrium model to cover a certain energy demand.

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Table 4.2 – continued from previous page

MACROECONOMIC AND POLICY MODEL	
Question	**Answer**
How is the capital stock modelled?	For TEA: "Capital stock evolves at each period with the formation of new capital that depends on the investment level in that period and the capital depreciation rate", for COFFEE, there are three possibilities depending on the technology: 1- Single capital stock with fixed lifetime and load factor, early retirement via reduction in load factor possible, 2- Capital vintaging with fixed lifetime and load factors, early retirement of vintages or reduction in load factors possible, 3- Single capital stock with fixed lifetime and load factor, without early retirement.[c]
How is depreciation of capital stock modelled?	In TEA, it is modeled by a depreciation rate given by model calibration run after the input of macroeconomic data given in GTAP. In COFFEE, fixed lifetimes are assumed for all energy infrastructures.[c]
How are prices determined?	In TEA, prices are endogenous and obtained after optimization. Initial prices and constants from elasticity curves are provided to calibrate the model. In COFFEE, energy and carbon prices are system inputs that can come from the CGE or another macroeconomic scenario generator.[b, c]
How is global trade modelled?	Quantities of energy are traded between the defined 18 world regions assessed in the COFFEE results. Imports and exports are defined for primary, secondary, and final energy for all different types.[b]

[a]Source: Annex III AR6 of WGIII IPCC (2022)
[b]Source: ROCHEDO (2016)
[c]Source: CUNHA *et al.* (2020)

4.1.1.3 Energy Conversion

Table 4.3: Energy Conversion Structure

ENERGY CONVERSION STRUCTURE	
Question	**Answer**
How is the split into different energy conversion technologies modelled?	Via least marginal cost optimization under given expansion constraints.[a]
How are the costs for energy conversion and their change over time modelled?	CAPEX and OPEX of energy converters are provided exogeneously. Technological changes, public policies, among others, can be translated into changes in these prices.[b, a]
What life cycle stages (construction, operation/maintenance, demolition) of energy conversion installations are considered?	The cost of the whole lifecycle is considered into the LCOE, including construction, operation, maintenance and decommission/demolition.[b]

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Table 4.3 – continued from previous page

ENERGY CONVERSION STRUCTURE	
Question	**Answer**
How are investment decisions into different energy conversion technologies modelled?	Via least marginal cost optimization under given expansion constraints (emission constraints imposed by each carbon budget scenario).[a]
How is the aging of different energy conversion technologies modelled?	It is modelled in three different ways depending on the technology on policy scenarios: 1- Fixed lifetime and load factor, early retirement via reduction in load factor possible, 2- Vintaging with fixed lifetime and load factors, early retirement of vintages or reduction in load factors possible, 3- Fixed lifetime and load factor, without early retirement.[a]
How is the service provided by the energy conversion installations described?	The model represents the main conversion technologies with a high level of detail. Conversion factors between energy services and secondary and primary energies are used to obtain the total primary energy.[b]
How is the capacity/utilization factor of the different installations determined?	Total availability of power generation plants are modeled on an annual basis. Typical maintenance stop times, unavailability due to technological limitations, as well as unavailability factors due to environmental issues in the case of renewables are considered.[b]

[a]Source: Annex III AR6 of WGIII, IPCC (2022)

[b]Source: ROCHEDO (2016)

4.1.1.4 Transportation Sector

Table 4.4: Transportation Sector Structure

TRANSPORT SECTOR STRUCTURE	
Question	**Answer**
How is the total demand for transport modelled?	”The main input data used is based on a model from the International Council on Clean Technology (ICCT, 2012). It is an open source software exclusively for the global transportation sector. The ICCT’s Global Transportation model is a tool developed to help policy makers worldwide identify and understand trends in the transportation sector, assess emission effects of different policy options, and frame plans to effectively reduce emissions of both greenhouse gases (GHGs) and local air pollutants. The model has a lot of input data... the input of socioeconomic data, such as GDP and population, were modified in order to estimate the future demand of energy services. The model has a series of econometric methods in order to estimate the demand of energy services for transportation of passengers (PKM) and freight (TKM).” [a]

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Table 4.4 – continued from previous page

TRANSPORT SECTOR STRUCTURE	
Question	**Answer**
How is the split into different transport modes modelled?	The ICCT model incorporates a large array of input data that has not been altered. This data includes region-specific average passenger occupancy (passengers per vehicle), typical mileage (km per year), historical fleet by region, and fleet composition by type and technology, among others. The economic input data of the model (such as GDP, population, and prices based on IEA scenarios) are then adapted to match those used in COFFEE, while maintaining the constants of the Gompertz demand elasticity curves used in the model which serve to calculate future service demand. In order to explore mitigation scenarios, options for shifting from less efficient to more efficient modes, as well as new technologies, have been added to the ICCT model. [a]
How are the costs for different transport modes and the change of modal split over time modelled?	Costs are exogenously given depending on the scenario narrative studied. ICCT provides the transport service demand over the run period as well as the initial fleet, COFFEE is thus responsible for suggesting different technologies within the same mode, although it does not internally address modal shifting. [a,b]
What life cycle stages (construction, operation/maintenance, demolition) of transport equipment are considered?	Usually not considered. Some study cases input additional costs to electric cars to assess grid reinforcement due to their use and battery disposal costs. [a,c]
How are investment decisions into different modes of transport modelled?	Mostly based on optimization costs and caps and trade policies introduced. Other restrictions are also inputted in order to create feasible scenarios (e.g., not every passenger using electric trains, etc). [c]
How is the aging of different vehicles/aircrafts/... modelled?	Not considered. [a]
How is transport service described?	By pkm and tkm services using the ICCT model. "The model has a series of econometric methods in order to estimate the demand of energy services for transportation of passengers (PKM) and freight (TKM). Based on the analysis of historical data, the model uses a constant elasticity for mobility per capita relative to income and population. In simple terms, the population projections are used in combination with GDP and relative fuel price forecasts, taken from the scenarios within IEA (2011), to predict future transportation activity. The relationships between these factors are assessed through a series of Gompertz functions." [a]
How is the capacity/utilization factor of the different vehicles/aircrafts … modelled?	The model provides regional information on occupancy factor (passenger per vehicle) and typical mileage (km per year) for every transportation mode, as well as efficiency and fleet composition in terms of fuel and technology used. Just as for the passenger technologies, the ICCT model provides regional data on occupancy and typical mileage for all three truck sizes and rail. [a]

Continued on next page

Table 4.4 – continued from previous page

TRANSPORT SECTOR STRUCTURE	
Question	**Answer**
How is the energy demand of transportation described?	Transport service is translated into secondary and primary energy using conversion factors that depend on the technology chosen by COFFEE. [a]
How is the material demand of transportation described?	With the exception of the demand for fuels, there is no description of the demand for materials for the sector. [a]

[a]Source: ROCHEDO (2016).
[b]Source: CALLEGARI (2021).
[c]Source: Class notes from COFFEE lecture.

4.1.1.5 Infrastructure Sector

Table 4.5: Infrastructure Sector Structure

INFRASTRUCTURE SECTOR STRUCTURE	
Question	**Answer**
How is the total demand for infrastructure modelled?	Non-energy infrastructure is not represented in COFFEE.[b]
How are the cost for infrastructure over time modelled?	Refer to the cost of energy infrastructure as other infra are not represented in the model.[b]
What life cycle stages (construction, operation/maintenance, demolition) of infrastructure are considered?	Refer to the cost of energy infrastructure as other infra are not represented in the model.[b]
How are investment decisions into infrastructure modelled?	Refer to the investment decision of energy infrastructure as other infra are not represented in the model.[b]
How is the aging of infrastructure modelled?	Refer to the aging of energy infrastructure as other infra are not represented in the model.[b]
How is infrastructure service described?	Not described.[b]
How is the capacity/utilization factor of infrastructure modelled?	The refining model, CAESAR, operates with certain utilization factors depending on fuel demand. The capacity factors are provided by coefficients from the literature.[b]
How is energy demand of infrastructure described?	
How is material demand of infrastructure described?	Not described.[b]

[b]Source: ROCHEDO (2016)

4.1.1.6 Buildings Sector

Table 4.6: Buildings Sector Structure

BUILDINGS SECTOR STRUCTURE	
Question	**Answer**
How is the total demand for buildings modelled?	Historical values of inhabitants per dwelling were employed for residential buildings. To assess changes in these values over time, a correlation was established between household expenditure and them. Both household expenditure (HHE) and population are externally provided from the energy model. For non-residential buildings, demand was computed based on floor space using a correlation between GDP and it.[b]
How is the split into different building types modelled?	Energy demand is aggregated into two building categories, residential and non-residential.[b]
How are the cost for different building types and the change of type split over time modelled?	Not described
What life cycle stages (construction, O&M, demolition) of buildings are considered?	Not described
How are investment decisions into different types of buildings modelled?	Not described
How is the aging of different building types modelled?	Not described
How is the service provided by buildings described?	Just energy service demand is described using the same categories used by IEA, which are: Space Heating, Water Heating, Cooking, Lighting, Cooling (Ambient Conditioning), and Appliances. This energy services are then aggregated into fuel and electricity.[b]
How is the capacity/utilization factor of the different building types modelled?	Not described
How is energy demand of buildings described?	For residential buildings, total dwelling demand is multiplied by the energy vector demand per dwelling disaggregated, as previously mentioned. In order to assess the influence of the regional weather on residential energy service, two additional indicators were used: Heating Degree-Days (HDD) and Cooling DegreeDays (CDD). For non-residential buildings, the same methodology is used, but the energy vector is given in energy per floor area, instead of energy per dwelling.[b]
How is material demand of buildings described?	Material demand for buildings is not modelled

Continued on next page

Table 4.6 – continued from previous page

BUILDINGS SECTOR STRUCTURE	
Question	**Answer**
How are appliances modelled?	It is modeled as a category of energy service demand for residential buildings/households. Appliances represent one of the energy demands in the residential sector, estimated in terms of energy services. This demand is calculated using the IEA database and is expressed in Energy per dwelling or energy per floor area[b]
How is domestic hot water use and generation modelled?	It is modeled as a category of energy service demand for residential buildings/households. It uses the same methodology as for appliances.[b]
How is lighting in buildings modelled?	It is modeled as a category of energy service demand for residential buildings/households. It uses the same methodology as for appliances.[b]

[b]Source: ROCHEDO (2016), Chapters 5.5 and 5.6

4.1.1.7 Recycling and Waste Management Industries

Table 4.7: Recycling and Waste Management Industries

RECYCLING AND WASTE MANAGEMENT INDUSTRIES STRUCTURE	
Question	**Answer**
How is the total volume of waste modelled?	For Municipal Solid Waste (MSW), a correlation is made between household expenditure (HHE) and the mass of waste generated per capita per year. The evolution of economic indicators causes variation in per capita waste generation. Additionally, for each region, a percentage composition of this waste is estimated, divided into organic, paper, plastic, metal, and other categories. For agricultural waste, three factors are applied to the total agricultural production, resulting in three possible scenarios for waste mass generated: "theoretical, which accounts for all aboveground straw and stalk; ecological, which excludes the necessary residue to prevent environmental degradation; and available, which excludes the use of residues as livestock feed."[a]
How are the major recycling/downcycling loops modelled?	For MSW, it is assumed that part is converted to Waste-to-Energy (W2E). For agricultural waste, it is considered that any non-decomposed waste is used for energy generation or burned. There is a nuclear generation technology, the Fast Breeder Reactor using UO_2 with reused plutonium dioxide; however, the recycling cycle of this fuel is not taken into account. Iron recycling is modeled solely as a maximum percentage of annual demand that can be met through this route, with associated GHG emissions and financial costs.[a,b]

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Table 4.7 – continued from previous page

RECYCLING AND WASTE MANAGEMENT INDUSTRIES STRUCTURE	
Question	**Answer**
How are the costs for different waste treatment options and the change of split of waste streams across treatment methods over time modelled?	Not modelled[a]
What life cycle stages (construction, operation/maintenance, demolition) of waste treatment installations are considered?	Not considered[a]
How are investment decisions into different types of waste treatment modelled?	Not considered[a]
How is the aging of different waste treatment installations modelled?	Not considered[a]
How is the capacity/utilization factor of the different waste treatment installations modelled?	Not considered[a]
How is energy demand of waste treatment described?	Not modelled explicitly[a]
How is material demand of waste treatment described?	Not described[a]

[a]Source: ROCHEDO (2016)

[b]Source: ZOTIN (2024)

4.1.1.8 Industries and Material Production

Table 4.8: Industries and Material Production

INDUSTRIES AND MATERIAL PRODUCTION STRUCTURE	
Question	**Answer**
How is the total demand for materials modelled?	Modelled for primary energy suppliers (oil, coal, uranium, NG), cement, Iron & steel, chemicals (HVC, ammonia, methanol and others). The demand for industrial products is determined by economic relationships via GDP or GDP per capita and is provided by the CGE model or another macroeconomic scenario generator. COFFEE optimizes energy demand to meet industrial demand. Thus, the demand for previously described industrial materials is supplied through a top-down approach, while the demand for energy materials is handled via a bottom-up approach.[a,b]

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Table 4.8 – continued from previous page

INDUSTRIES AND MATERIAL PRODUCTION STRUCTURE	
Question	**Answer**
How is steel production and recycling modelled?	The demand is calculated through economic relationships as mentioned above. Iron and steel production is modeled through 14 technologies that can be grouped into 3 types: integrated routes, sponge iron routes, and electric arc furnace routes, including some with CCS. The input can be either iron ore or scrap. Maximum regional limits for meeting demand with scrap have been set. Each route has an associated energy demand and a GHG emission. Costs include installation and O&M. The model optimizes supply based on the lowest cost, considering the imposed constraints. A better description of this module can be seen in ZOTIN (2024)[b]
How is cement production modelled?	The modeling of demand and supply is analogous to that of iron and steel. For cement, production is divided into three parts: HTH (High Temperature Heating) generation with 6 energy sources, each with and without CCS; clinker production through four routes; and, finally, cement production by adding various cementitious materials to the clinker mix[b]
How is chemicals production modelled?	In COFFEE, the chemical sector is modeled with a division between a technology-rich sector, which includes High Value Chemicals (HVC), methanol, and ammonia, and an aggregated sector covering the remainder. The HVC sector can be subdivided into co-production, multiproduct, and on-purpose routes, totaling 21 possible pathways. It is important to note that the first two routes have a strong correlation with the hardware of the 5 refinery typologies described in COFFEE, as chemical production by these groups may increase or decrease depending on the type and configuration chosen for the refineries. For methanol, 7 possible routes are modeled, 3 of which include CCS, and for ammonia production, 8 routes for H_2 production are modeled prior to the Haber-Bosch synthesis.
How are other metals modelled?	Not explicitly modelled[b]
How is competition/substitution between materials modelled?	In some sectors, the source of raw materials can be substituted, especially with biomass. Some substitutions analyzed include sugar-cane-derived ethanol to ethylene (with and without CO_2 capture and storage – BECCS) or bio-methanol to ethylene. In refineries, chemical production competes with fuel production. Finally, biomass production also competes with food production in the land use module.[c,b]
How are the costs for different materials and the change of costs over time modelled?	Costs include an implementation cost and fixed and variable O&M values. Fixed costs remain constant over time, while variable costs, such as energy prices, input costs, and CO_2 costs, may vary over time depending on the macroeconomic scenario used.[b]

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Table 4.8 – continued from previous page

INDUSTRIES AND MATERIAL PRODUCTION STRUCTURE	
Question	**Answer**
How are investment decisions into different types of material production assets modelled?	Through cost optimization subject to scenario constraints. As with energy assets, it is possible to discontinue an operational asset and replace it with another or reduce its capacity factor.[b]
How is the aging of different material production assets modelled?	Through a fixed lifespan.[b]
How is the capacity/utilization factor of the different material production assets modelled?	Through cost optimization subject to scenario constraints. As with energy assets, it is possible to discontinue an operational asset and replace it with another or reduce its capacity factor.[b]
How is energy demand of material production described?	Through a mixed bottom-up and top-down approach. Demand is well-modeled for the industries described in COFFEE (cement, iron and steel, chemicals, and plastics); for these, production routes are detailed, as well as the energy demand for each. For industries classified as "other," demand is provided via a top-down approach, following pre-established economic relationships.[b,a]
How are other industries and energy end uses modelled?	To ensure complete coverage, an "Other Industries" sector was introduced in COFFEE to represent the energy use and emissions of industrial sectors not explicitly modelled... The residual energy use in the industrial sector was then allocated to the "other industries" sector. For simplicity, we assumed that the residual industrial energy use would grow at a rate comparable to that of the cement sector.[b]
What types of co-production/ industrial symbiosis are considered?	Refer to the question about chemicals and competition/substitution

[a]Source: ROCHEDO (2016)
[b]Source: ZOTIN (2024)
[c]Source: OLIVEIRA *et al.* (2020)

4.1.1.9 Land Use Model and Natural Resources

Table 4.9: Land Use Model and Natural Resources

LAND USE MODEL AND NATURAL RESOURCES STRUCTURE	
Question	**Answer**
How is the capital requirement in agriculture and other land management activities modelled?	The cost of agricultural and livestock production is determined by a combination of two factors: land productivity and the distance from the land to production sale points.[a]

Continued on next page

Table 4.9 – continued from previous page

LAND USE MODEL AND NATURAL RESOURCES STRUCTURE	
Question	**Answer**
How is the transportation demand in agriculture and other land management activities modelled?	The transportation demand for agriculture was estimated using a proxy for distance based on a georeferenced map from UNEP. Depending on the distance, a transport mode was assigned (truck, train, ship, or a combination). However, this demand is used solely to determine production costs and not to form energy services for transportation.[a]
How is the fertilizer demand in agriculture and other land management activities modelled?	Just transportation cost is modelled, as mentioned above.[a]
How is water use and supply modelled?	For the national model, BLUES, water withdrawal and consumption are explicitly modeled by energy generation source type and by type of crop or agricultural production. The other sectors modeled in BLUES using a top-down methodology include urban and rural human supply and industrial supply. Water availability is based on basin resources according to official data from Brazilian public agencies. There is a future perspective to implement part of this modeling in COFFEE, the global model.[b,c]
Other structure not covered elsewhere	None
How is resource depletion modelled?	Via resource supply curves, only for energy resources. Over time, lower-cost reserves are depleted, and higher-cost reserves come into use.[a]
How does resource depletion affect resource prices?	The supply curves relate a certain quantity of the assessed resource with a determined price. Over time, lower-cost reserves are depleted, and higher-cost reserves come into use. Only for energy resources.[a]
How does the constraint on land area feed back into the other parts of the model?	Increasing the production costs of biomass for energy generation and for non-energy products in the chemical industry.[a,d]
How does the constraint on exhaustible resources enter the other parts of the model?	This primarily increases downstream energy production costs of the depleted resources and drives the model to opt for cheaper energy sources.[a]
How does the constraint on the throughput/area for non-exhaustible resources enter the other parts of the model?	Via resource supply curves. Supply curves for renewable relate potential in PWh/year vs LCOE. Learning rates for some technologies affect supply curves by increasing total available potential and reducing costs.[a,e]

[a]Source: ROCHEDO (2016)

[b]Source: ANGELKORTE (2023)

[c]Source: ARROYO (2018)

[d]Source: ZOTIN (2024)

[e]Source: CUNHA *et al.* (2020)

4.1.2 Resolution Details

4.1.2.1 General Model Setup

Table 4.10: General Model Setup

GENERAL MODEL SETUP	
Question	**Answer**
What is the time frame of the model?	2010-2100.[a]
What are the time steps of the model?	5 year steps until 2050 and 10 year steps from 2050 until 2100[a]
Which economic regions are considered?	18 regions (AFR - Africa, AUS - Australia and New Zealand, BRA - Brazil, CAM - Central America, CAN - Canada, CAS - Caspian Region, CHN - China, EEU - Europe, IND - India, JPN - Japan, KOR - South Korea, MEA - Middle East, RAS - Rest of Asia and Oceania, RUS - Russia, SAF - South Africa, SAM - South America, USA - United States, WEU - Rest of Europe)[a,b]
What is the time horizon of the optimization (foresight)?	In COFFEE, it is perfect foresight until 2100.[c]

[a]Source: IAMC (2020)

[b]Source: ROCHEDO (2016)

[c]Source: KEPPO *et al.* (2021)

4.1.2.2 Macroeconomic and Policy Model

Table 4.11: Macroeconomic and Policy Model

MACROECONOMIC AND POLICY MODEL	
Question	**Answer**
Which factors of production are considered?	TEA: The main variables of the macro-economic model are capital stock, available labour, available land, and available natural resources and intermediates (for agriculture, energy, industry, transport, and services). Energy sectors are divided into coal, crude oil, electricity, natural gas, and petroleum coal products. COFFEE: Land and energy resources. [a,b]
Which lifetime distribution of the capital stock is used?	Both COFFEE and TEA assume constant lifetime for energy assets. They do not take into account existing stock and future demands in the transportation, building, and industrial sectors. [a,b]
Which (climate) policy interventions are included?	Structural changes of the energy system, replacement of fossil fuels, price-induced changes of demand. Renewable technologies, alternative conversion processes, CCS, bioenergy. Also carbon prices, GHG taxes, GHG emission cap and permit trading, subsidies, and regulations. [c]

Continued on next page

Table 4.11 – continued from previous page

MACROECONOMIC AND POLICY MODEL	
Question	**Answer**
What are the types of capital stock considered?	Electric power generation infrastructure, industrial infrastructure for cement, steel, and chemicals, refining infrastructure, and land. [b,d]

[a]Source: CUNHA *et al.* (2020).
[b]Source: ROCHEDO (2016).
[c]Source: Annex III AR6 of WGIII IPCC (2022).
[d]Source: ZOTIN (2024).

4.1.2.3 Energy Conversion

Table 4.12: Energy Conversion Resolution

ENERGY CONVERSION RESOLUTION	
Question	**Answer**
What are the primary energy carriers?	COFFEE: Oil, coal, natural gas, uranium, sunlight, biomass, wind, geothermal, hydro. TEA: Coal, Crude oil, Natural Gas, Petroleum (Wind, sunlight, hydro, and geothermal are modeled into the Electricity Sector).[a]
What are the conversion technologies from primary to secondary energy carriers covered?	More than 100 electric generation technologies, including CCS options. More than 20 energy sources for the electric sector (3 types of oil derivatives, natural gas, 3 types of coal, 3 types of renewables, 8 types of nuclear fuels, PV, CSP, hydro, geothermal, wind). Refinery conversion is also represented by an auxiliary model, CAESAR, which produces refinery gas, LPG, Naphtha, Gasoil, Coke, and Fuel Oil depending on the type of refinery run, which can be Naphtha run, Diesel run, or Kerosene run. The model represents these outputs through an estimation of global refining capacity in various refinery units, which include: ACU – Atmospheric Distillation; VCU – Vacuum Distillation; ASP – Asphalt; FCC – Fluid Catalytic Cracking; ALQ – Alkylation; CRU – Catalytic Reforming; TCU – Thermal Cracking; HCC – Hydrocracking; DCU – Delayed Coking; HDT – Hydrotreating; LUB - Lubricant. Utilities in refinery are also assessed in this model: H2, steam, heat, FCC coke, and electricity.[a,b]
What are the secondary (final) energy carriers?	Electricity, Heat, Solid/Liquid/Gaseous fuel including biomass.[a,b]
What are the end-use sectors?	Transportation, Residential, Service, Industries, Agriculture, and Waste Sectors.[a]

Continued on next page

Table 4.12 – continued from previous page

ENERGY CONVERSION RESOLUTION	
Question	**Answer**
What are the industrial sectors covered?	Cement, Iron & Steel, Plastics/Chemicals, and the rest aggregated in "others Industries". Additionally, an industrial non-energetic demand of energy products are supplied by: Bituminous Coal, Sub-bituminous Coal, Lignite, Natural Gas, Liquefied Petroleum Gas, Gasoline (Naphta), Kerosene, Diesel, Fuel Oil, Petroleum Coke, Biomass, Charcoal, Electricity, Heat.[a,c]

[a]Source: ROCHEDO (2016).

[b]Source: Class notes from COFFEE lecture.

[c]Source: ZOTIN (2024).

4.1.2.4 Transportation Sector

Table 4.13: Transport Sector Resolution

TRANSPORT SECTOR RESOLUTION	
Question	**Answer**
Which transport modes are covered (freight and passenger)?	COFFEE, based on the ICCT model, split transport modes for passengers into the following ones: cars, 2 wheels, 3 wheels, buses, trains, and planes. For freight: small, medium and heavy trucks, ships, and trains. Cars have their technological split into ICE, Flex Fuel, Hybrid, plug-in Hybrid, battery and Fuel Cell electric cars. Buses are split into conventional and ethanol buses. Trains into conventional and electrical trains. Trucks into conventional, efficient (fossil-based), and ethanol. Finally, ships into conventional and efficient ones. In terms of fuels, most of the options are related to road vehicles, which include: diesel (conventional, low-sulphur), ethanol (grain, sugarcane, cellulosic), biodiesel (oil-based, lingo-cellulosic), Natural Gas, LPG, hydrogen, electricity, jet fuel, and fuel oil. [a]
What energy carriers are considered in transportation?	Diesel (conventional, low-sulphur), ethanol (grain, sugarcane, cellulosic), biodiesel (oil-based, lingo-cellulosic), Natural Gas, LPG, hydrogen, electricity, jet fuel, and fuel oil. [a]
What materials are considered in transportation?	None, except for the fuels. [a]

Continued on next page

Table 4.13 – continued from previous page

TRANSPORT SECTOR RESOLUTION	
Question	**Answer**
What drive technologies and other transport technologies are covered?	Price and emission restrictions. Some mitigation options were introduced into the ICCT model. The first one is related to a shift in transportation modes between less efficient to more efficient ones; shifts from LDV to buses for passengers and from heavy trucks to trains for freights. The second one was the introduction of alternative technologies like electric and fuel-cell vehicles. The third one is the choice between fossil-based or ethanol trucks. The fourth is the split between electric and conventional trains, and, last, the division between conventional and efficient ships. [a]
[a]Source: ROCHEDO (2016)	

4.1.2.5 Infrastructure Sector

Table 4.14: Infrastructure Sector Resolution

INFRASTRUCTURE SECTOR RESOLUTION	
Question	**Answer**
What infrastructure types are covered?	Electric power generation infrastructure, industrial infrastructure for cement, steel, and chemicals, refining infrastructure. [a,b]
What energy carriers are considered for infrastructure?	Specified in the Energy Conversion section. [a]
What materials are considered for infrastructure?	None. Although COFFEE describes the infrastructure required to meet an aggregated demand, the specific demand for the infrastructure sector is not considered separately. [a,b]
[a]Source: ROCHEDO (2016). [b]Source: ZOTIN (2024).	

4.1.2.6 Buildings Sector

Table 4.15: Buildings Sector Resolution

BUILDINGS SECTOR RESOLUTION	
Question	**Answer**
What building types are covered?	Residential and non-residential (service) buildings, but only their energy demand (in COFFEE). For both sectors, the demand is calculated using the IEA database, which provides energy demand proxies either per dwelling or per m^2. The demand is divided into six types: space heating, water heating, cooling, lighting, appliances, and cooking. There is no segmentation into different building types, only an aggregated demand that can vary over time depending on changes in macroeconomic parameters.[a]

Continued on next page

Table 4.15 – continued from previous page

BUILDINGS SECTOR RESOLUTION	
Question	**Answer**
What energy carriers are considered for buildings?	Energy service for residential and service buildings are: Space Heating, Water Heating, Cooking, Lighting, Appliances, and Cooling that can be provided by fuels and/or electricity.[a]
What materials are considered for buildings?	None.[a]
What types of appliances are considered?	Appliances are not modeled explicitly, just their energy demand.[a]
What types of lighting for buildings are considered?	Separated into electric and non-electric demand (kerosene, candles, others).[a]
What types of heating systems for buildings are considered?	They are not explicitly modeled.[a]
What types of hot water generation for buildings are considered?	They are not explicitly modeled.[a]
What other building technologies are considered?	None, just the sector's aggregated energy demand is modeled.[a]
[a]Source: ROCHEDO (2016)	

4.1.2.7 Recycling and Waste Management Industries

Table 4.16: Recycling and Waste Management Industries Resolution

RECYCLING AND WASTE MANAGEMENT INDUSTRIES RESOLUTION	
Question	**Answer**
What waste types are covered?	Municipal Solid Waste (MSW) and Agriculture residues [a]
What recycling systems are covered?/ For which materials is recycling modelled?	MSW can be disposed of in Dumps, Landfills, Compost, Incineration, Recycled, or used as Waste to Energy (W2E). Emissions for each of the first five disposal options are evaluated, while the last option is considered as a potential energy resource. For agricultural residues, a "yield" was assigned to each type of crop. From the total residue available, the ecological portion, which serves to prevent environmental degradation, and the portion used for animal feed were subtracted. The remainder is considered biomass available for the energy sector. [a]
What waste treatment processes are considered?	As cited above [a]
What recycling technologies are considered?	None [a]
[a]Source: ROCHEDO (2016).	

4.1.2.8 Industries and Material Production

Table 4.17: Industries and Material Production Resolution

INDUSTRIES AND MATERIAL PRODUCTION RESOLUTION	
Question	**Answer**
What material production industries are covered?	Cement, Iron & steel, Chemicals and others. Emissions for each sector are considered separately. [a,b]
What production technologies are considered for the different materials?	The routes for cement, steel and chemicals production are detailed in II [b]
What other industries/end use sectors are covered?	Only the ones previously covered [c]
What energy carriers are considered for other industries/end use sectors?	None [c]
What materials are considered for other industries/end use sectors?	None [c]
[a]Source: Class notes from COFFEE lecture. [b]Source: Tese Marianne ZOTIN (2024). [c]Source: Tese Pedro ROCHEDO (2016).	

4.1.2.9 Land Use Model and Natural Resources

Table 4.18: Land Use Model and Natural Resources Resolution

LAND USE MODEL AND NATURAL RESOURCES RESOLUTION	
Question	**Answer**
Which non-exhaustible primary energy resources are covered?	Bio-energy, solar (thermal, concentrated solar power, PV), hydro, wind, geothermal [a]
Which exhaustible primary energy resources are covered?	Coal, conventional/unconventional gas and oil, uranium [a]
Which natural resources other than primary energy carriers are considered?	Land [a]
What mineral resources are modelled?	None except for the energy resources [a]

Continued on next page

Table 4.18 – continued from previous page

LAND USE MODEL AND NATURAL RESOURCES RESOLUTION	
Question	**Answer**
What are the throughput/area constraints for the non-exhaustible resources?	For energy resources, supply curves per cost are applied. Supply curves for renewable resources relate potential in PWh/year vs. LCOE. Data is based on IRENA and NREL. Learning rates for technologies affect supply curves, increasing total potential and reducing costs. Constraints like national reserves are excluded for hydro and geothermal exploitation. For bio-fuels, economic values for land are assigned by combining land cover category, soil productivity, and distance from consumption centers. Constraints are imposed through price and carbon restrictions. Different yields are assigned per area for each crop and livestock type. [a]
What are the global supply caps for exhaustible primary energy carriers?	One of the initial steps of COFFEE was to create an inventory of probable reserves of natural gas, oil, coal, and uranium. These resources are allocated in supply-demand curves; for more details, see ROCHEDO (2016) and DE OLIVEIRA (2021). [a,b]
What are the global supply caps for other exhaustible resources?	For land use, economic values for each area are assigned by combining three factors: land cover category, soil productivity, and distance from consumption centers. Constraints are imposed through price and carbon emission restrictions. [a]
What types of fertilizer are modelled?	Although the synthesis of ammonia and urea is evaluated within the chemicals segment of the industrial sector, there is no specific assessment of fertilizers. [c,a]
What types of water (green, grey, ...) are modelled?	For the national model, BLUES, water withdrawal and consumption are explicitly modeled by energy generation source type and crop type. Other sectors modeled include urban and rural human supply and industrial supply. Water availability is based on basin resources according to Brazilian public agencies. Part of this modeling is planned for COFFEE. [d,e]
What land use types are modelled?	The following land use types are modeled: Forest, Pasture, and Cropland. Transitions between these types follow specific rules. Additionally, land cover is categorized into seven types combined with soil productivity indices and distances to classify into six economic categories. [a]
What is the spatial resolution of the land use model?	9ha (0.09km^2) per land sector, not geographically explicit. [a]

[a]Source: ROCHEDO (2016).
[b]Source: DE OLIVEIRA (2021).
[c]Source: ZOTIN (2024).
[d]Source: ARROYO (2018).
[e]Source: ANGELKORTE (2023).

Table 4.19: Climate and Ecosystem Linkages

CLIMATE AND ECOSYSTEM LINKAGES	
Question	**Answer**
Which direct GHG are considered?	CO_2, CH_4, N_2O [a]
Which non-GHG forcing agents are considered?	None [a]
With other emissions to the environment (pollutants, indirect GHG, ...) are considered?	None [a]

[a]Source: Annex III of the AR6 of WGIII IPCC (2022).

4.2 Structured description of ODYM-RECC

This section analyzes the inputs and outputs of ODYM-RECC as described in the methodology. The analysis considers an integration between the model and a generic technology-rich IAM. The specific analysis and integration proposal with COFFEE will be addressed later.

To understand the inputs and outputs of ODYM-RECC, it is essential first to grasp the structure of the dMFA system within its code framework. The three main libraries of the ODYM framework are the classes library, the functions library, and the dynamic stock model library. These are imported with the following sequence of Python codes:

```
import ODYM_Classes as msc  # Import the ODYM class file
importlib.reload(msc)
import ODYM_Functions as msf  # Import the ODYM function file
importlib.reload(msf)
import dynamic_stock_model as dsm  # Import the dynamic stock
 model library
importlib.reload(dsm)
```

The functions of the ODYM library will not be explored in depth; it is worth noting, however, that they are responsible for performing calculations of flow variations, stock levels, mass balance closure, among other operations, after the system has been fully declared.

The dMFA system is declared and allocated using the functions within the `dsm` library. To do this, a list of processes and dictionaries of flows, stocks, and parameters must be created (see 2.15). Below is the definition of a generic dMFA:

```
Dyn_MFA_System = msc.MFAsystem(Name = 'TestSystem',
Geogr_Scope = 'TestRegion',
```

```
    Unit = 'Mt',
    ProcessList = [],
    FlowDict = {},
    StockDict = {},
    ParameterDict = {},
    Time_Start = Model_Time_Start,
    Time_End = Model_Time_End,
    IndexTable = IndexTable,
    Elements = IndexTable.loc['Element'].Classification.Items) # Initialize MFA system
```

Taking processes as an example, through the `msc.Process` class, it is necessary to provide a name, a number, and link the aspects (time, region, products, etc., see Figure 2.13) of the process. These various processes are then aggregated into a list. The list of all processes in ODYM-RECC is shown in Figure 2.14.

For parameters, such as process yields, material intensities of goods, and many others, the `msc.Parameter` class is used. These are essentially those listed in Figure 2.15, with aspects also present in the table. These parameters are constituted by the data from Excel tables in the ODYM-RECC database, obtained from `https://zenodo.org/records/12752350` (PAULIUK, 2024). For them, a Python dictionary is created, which will serve as an input for initializing the dMFA. The same applies to flows, for which primarily the name, the connecting processes, and the aspects are declared. Below is a snippet of ODYM-RECC code that inserts three flows into the flow dictionary [1]:

```
RECC_System.FlowDict['F_4_5'] = msc.Flow(Name='primary material consumption', P_Start = 4, P_End = 5, Indices = 't,m,e', Values=None, Uncert=None, Color = None, ID = None, UUID = None)

RECC_System.FlowDict['F_5_6'] = msc.Flow(Name='manufacturing output', P_Start = 5, P_End = 6, Indices = 't,o,g,m,e', Values=None, Uncert=None, Color = None, ID = None, UUID = None)

RECC_System.FlowDict['F_6_7'] = msc.Flow(Name='final consumption', P_Start=6, P_End=7, Indices='t,r,g,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
```

Taking the last declared flow as an example, it connects processes 6 (market for consumer goods, buildings, vehicles, etc.) and 7 (use phase). It is called *final consumption* and includes the aspects t (time), r (region), g (goods), m (engineering materials), and e (elements).

Finally, a dictionary of stocks and stock changes is declared. More than one stock can be associated with a single process. A stock can have various aspects in

[1] flows are defined from line 1158 until 1313 in ODYM-RECC code

its declaration, and each aspect will have a data vector. For instance, the stock of process 7, *use phase*, includes the aspects t, c, r, g, m, e (time, cohort, region, good, material, and element). The *good* aspect, for example, has 37 types, resulting in a vector with 37 positions. This enables segregation to determine how much of a specific good g_{20} was present in region r_3 at time t_1, as well as the corresponding amount of a specific element e_2 and material m_5 in stock.

To facilitate the presentation of results, the modeler can choose to separate the stocks of a process. Below is a code snippet that shows the declaration of the stock for process 7, its variation, and the segregation of the stock in process 1:

```
RECC_System.StockDict['dS_1t'] = msc.Stock(Name='Forestry stock change, timber', P_Res=1, Type=1, Indices = 't,r,e', Values=None, Uncert=None, ID=None, UUID=None)

RECC_System.StockDict['S_1t'] = msc.Stock(Name='Forestry carbon stock, timber', P_Res=1, Type=0, Indices = 't,c,r,e', Values=None, Uncert=None, ID=None, UUID=None)

RECC_System.StockDict['dS_1f'] = msc.Stock(Name='Forestry stock change, fuel wood', P_Res=1, Type=1, Indices = 't,r,e', Values=None, Uncert=None, ID=None, UUID=None)

RECC_System.StockDict['S_1f'] = msc.Stock(Name='Forestry carbon stock, fuel wood', P_Res=1, Type=0, Indices = 't,c,r,e', Values=None, Uncert=None, ID=None, UUID=None)

RECC_System.StockDict['S_7'] = msc.Stock(Name='In-use stock', P_Res=7, Type=0, Indices = 't,c,r,g,m,e', Values=None, Uncert=None, ID=None, UUID=None)
```

The understanding outlined above is fundamental because the inputs to ODYM-RECC are essentially the parameters, which must be harmonized if part of them are received from the IAM.

In the case of outputs, knowing which variables are calculated in ODYM-RECC and how they are stored is the first step to identifying the model outputs that will feed the IAM and understanding their properties.

4.2.1 Analysis of ODYM inputs and necessary changes

The inputs were organized into a table containing the data and diagnostic questions listed in Section 3.2. For better readability, the tables have been included in Appendix III. There is little to add to the table. One of the comments is to reaffirm the need to adjust the temporal step, the regions, and the final year of the model. Another issue is that the integration heavily depends on the IAM with which it is intended to integrate. For instance, if the IAM does not include a material energy demand sector, it would be difficult for ODYM-RECC to contribute to the IAM in this regard. However, this does not preclude the possibility of establishing a one-way soft-link, where the dMFA model calculates the material demand for the given energy service demand.

4.2.2 Analysis of ODYM outputs and necessary changes

Unlike the inputs, which are primarily Excel files related to parameters, the outputs can vary and are broadly divided into two types. The first type consists of those calculated within the dynamic system itself, such as flows (inflows and outflows) and stocks (including stock levels and their variations) across various aspects. These outputs can be detailed to combine with any of the possible aspects (defined in the flow or stock declaration), such as region, industrial material, or time. Codes III.1 and III.2 in Annex III list all flows and stocks declared in the model.

The second type includes indirect calculations using the first type. For example, water usage for a specific inflow of a certain material. For this type, a results vector, such as the copper inflow over time, is multiplied by a parameter (input to ODYM-RECC), such as water consumption per mass of copper produced. This allows obtaining any result that combines a primary result (flow or stock) with a parameter, always with the option to detail by aspects. Code III.3 in Annex III lists all output vectors created. It is important to note that new outputs can be created, either using existing data in the current ODYM-RECC configuration or with new parameter inputs in future versions.

For the first type, the harmonizations that must be performed are related to region and temporal step, as discussed later. This is because these data are obtained specifically from a dMFA model, not from an IAM. An IAM may receive a consumption vector demand of a specific material as an input but does not generate it as a result of its run. If that is the case, ODYM-RECC can serve as the tool to provide that vector, with the mentioned adjustments applied, instead of receive it from a CGE or a scenario generator.

For the second type, two options exist. The first involves quantities evaluated within IAMs, such as atmospheric emissions, which are often calculated by sector or in aggregate. ODYM-RECC allows disaggregation to the product level if it has been declared in its configuration. The second involves less common results, such as water usage. For this second type, it is essential that the conversion factors, such as CO_2 generated per mass of cement produced, are consistent to ensure compatible final results. However, this factor is precisely an input to ODYM-RECC, as discussed in the previous section.

4.3 Integration between COFFEE and ODYM-RECC

ODYM-RECC currently has two major sectors described that are common to COFFEE: the building and the transportation sector. This section will analyze the compatibility required for integration between them, making some proposals.

To facilitate the analysis, tables 4.20 and 4.21 illustrate the level of detail for each sector in ODYM-RECC for the copper model, which has already included current ODYM-RECC v2.5 sectors and the new sectors.

Table 4.20: Resolution of sectors currently described in ODYM-RECC

TRANSPORT	**RESIDENTIAL BUILDINGS**	**NON-RES BUILDINGS**
Internal Combustion Engine gasoline (ICEG)	SFH non-standard	Offices
Internal Combustion Engine diesel (ICED)	SFH standard	Commercial
Hybrid Electric Vehicles (HEV)	SFH efficient	Educational
Plugin Hybrid Electric Vehicles (PHEV)	SFH ZEB	Health
Battery Electric Vehicles (BEV)	MFH non-standard	Hotels and Rest.
Fuel Cell Vehicles (FCV)	MFH standard	Others
	MFH efficient	
	MFH ZEB	
	RT non-standard	
	RT standard	
	RT efficient	
	RT ZEB	

Table 4.21: Resolution of sectors to be described in ODYM-RECC and already described in ODYM-COPPER (KLOSE and PAULIUK, 2023)

INDUSTRY	**APPLIANCES**	**INFRASTRUCTURE**	**TRANSPORT**
Solar PV power plant	Fan	Traffic lights	Electric motorcycles
CSP plant	Air-cooler	Street lights	Gasoline motorcycles
Wind power plant onshore	Air-conditioning	Conventional rail system	Diesel bus
Wind power plant offshore	Refrigerator	High-speed rail system	Hybrid bus
Hydropower plant	Microwave	MV overhead	Electric bus
Nuclear power plant	Washing Machine	Hv Substations	Trucks
Coal power plant	Tumble dryer	Mv Substations	Locomotive
Bio powerplant	Dishwasher	Lv Substations	Freight railcars, wagon
Oil power plant	Television	Hv Transformers	Freight railcars, railcars
Geothermal power plant	VCR/DVD player	Mv Transformers	Passenger rolling stock
Gas comb. cycle power plant	PC & Laptop	Lv Transformers	Vessels
Other industrial durables	Other small appliances	Other infrastructure	Aircrafts
Other agricultural durables	Other appliances	HV overhead	
	Diverse equipment	HV underground	
		MV underground	
		LV overhead	
		LV underground	

4.3.1 Integration for the Transportation Sector

4.3.1.1 Passenger Transportation

ODYM-RECC, by using the service outputs in pkm (passenger-kilometers) from IMAGE, needs to convert this final service into a vehicle fleet. For the passenger sector, it uses the following formula:

$$PKM_x = OR_x \cdot VKM_x \cdot s_x \tag{4.1}$$

where PKM_x is the passenger transport service in passenger-kilometers per year, OR_x is the average vehicle occupancy rate (passenger/vehicle), VKM_x is the annual mileage (km) per vehicle, and s_x is the stock (quantity) of active vehicles. The index x represents the subdivision of usage categories, which are as follows:

- Mobility by privately-owned and not shared vehicle stock (index 0)
- Mobility by car-shared but not ride-shared vehicle stock (index CaS)
- Mobility by ride-shared but not car-shared vehicle stock (index RiS)
- Mobility by car-shared and ride-shared vehicle stock (index CaS+RiS)

This is done to determine the total vehicle fleet. The subdivision into the four segments/archetypes (microcar, passenger car, minivan_SUV, and light truck, discussed in section 2.4.2.2) and the six technologies is then made depending on the simulated scenarios. Scenarios with higher Material Efficiency, use of smaller vehicles, as well as higher occupancy and sharing rates.

The following will describe how COFFEE handles transport service demand and possible integrations. As mentioned in the COFFEE diagnostic tables, the ICCT model provides the transport service demands in pkm and tkm to be met by COFFEE. The software also supplies the initial fleet composition through shares of vehicle types and technologies. Other important data provided include the average vehicle occupancy by region and annual mileage. Modifications were made to the ICCT model, which is built in open-source code, to adapt it to COFFEE: the first was regional harmonization from 11 to 18 regions; another was the inclusion of additional technological options, such as ethanol engines; a third was the possibility of substitution between modes.

During optimization, COFFEE seeks to meet the energy service demand by choosing among different technological pathways and associated fuels, depending on the input constraints and costs. However, it does not perform intermodal substitutions (CALLEGARI, 2021). Thus, any narrative regarding modal demand and shares provided by ICCT remains unchanged in the input. Therefore, as a first integration approach, ICCT results could be directly inputted into ODYM-RECC.

Since the ICCT model already provides the fleet composition, the calculation step described above can be avoided. Accordingly, some files from the database (see Appendix III) become unnecessary. These are (name and description):

1. `3_IO_Vehicles_UsePhase_v2.5.xlsx` (Annual vehicle kilometrage)
2. `6_MIP_VehicleOccupancyRate_V1.5.xlsx` (Occupancy rates for vehicles in different regions from 2015-2100)
3. `6_PR_CarSharingShare_V1.3` (Share of total passenger-km delivered by car-sharing)
4. `6_PR_RideSharingShare_V2.1` (Percentage of transport service demand fulfilled by ride-sharing from 2015 to 2100)
5. `3_SHA_DownSizing_Vehicles_V2.4` (Market share of each vehicle size segment, assumed to change annually from 2015 to 2100)
6. `3_SHA_LightWeighting_Vehicles_V1.4` (Market share of light-weighted vehicles per powertrain from 2015 to 2100)
7. `6_MIP_CarSharing_Stock_V1.0` (Ratio of per capita passenger vehicle stock with vs. without car-sharing)
8. `6_MIP_RideSharing_Occupancy_V1.1` (Occupancy rates for ride-sharing vehicles)

The following files should be retained but modified with ICCT data:

1. `2_S_RECC_FinalProducts_2015_passvehicles_V1.4 2015.xlsx` (Stock by age-cohort)
2. `1_F_Function_Future_V1.4` (Transport function to be fulfilled by the entire fleet, from 2015 to 2100, for each region)
3. `3_SHA_TypeSplit_Vehicles_V3.0` (Describes the split of vehicle types under different scenarios)

The files listed below, with the exception of additional harmonization discussed further on, such as regional compatibility, and additional data for different types of vehicles, can remain as they are. They primarily contain data on material intensities per vehicle archetype, flags for runs with different ME strategy configurations, and data calibration files that do not involve fleet size:

1. `3_El_Products_UsePhase_passvehicles_V1.3` (Operational energy demand, all energy carriers together)
2. `3_LT_RECC_ProductLifetime_passvehicles_V3.1` (Lifetime distribution parameters)
3. `3_MC_RECC_Vehicles_V1.1` (Material composition of stock)

4. `6_PR_LifeTimeExtension_passvehicles_V2.1` (Factor >= 1 that scales the current to the extended lifetime)
5. `6_PR_ReUse_Veh_V1.3` (Reuse rates for different materials (e.g., % of cast Al from reuse of vehicle components) in 6 vehicle archetypes, from 2015 to 2100, for each region)
6. `3_SHA_EnergyCarrierSplit_Vehicles_V1.1` (Splits total driving energy demand into different energy carriers for each vehicle technology)
7. `3_MC_VehicleArchetypes_V2.0` (Material composition of vehicle archetypes across different configurations)
8. `6_PR_Calibration_V2.5` Calibration values to scale energy intensity and vehicle operation
9. `8_FLAG_VehicleDownsizingDirection_V1.0` Flag set for scenario case to lead lower GHG emissions

There are two essential differences between the outputs of the ICCT model and the original inputs of ODYM-RECC: the vehicle type topologies used and the inclusion of ethanol-powered ICE (ICEE) technology in the ICCT model, which is utilized in COFFEE. For the first issue, the following tasks will need to be completed. The first is obtaining material intensity data for 2w and 3w vehicles, which are not described in ODYM-RECC. The second is gathering lifespan parameters for these vehicle types, including the probabilistic distribution and its parameters. A third point involves obtaining data on the existing fleet for model calibration and quantifying in-use stocks. Finally, estimating lifespan values for the currently existing fleet is needed to forecast the temporal output profile of existing stock and replacement requirements. Part of this data was collected by KLOSE and PAULIUK (2023), as shown in Table 4.21, although the material content described include only copper and other materials must be included, specially steel.

For the issue of ethanol ICE technology, the same approach as used for the other two ICE options, diesel and gasoline, is proposed: adopting the same material intensity and lifespan parameters. However, current fleet data will be used to recalibrate the model, though significant differences are unlikely, as Brazil is virtually the only country with a substantial fleet of vehicles with this technology.

It is important to note that the current version of ODYM-RECC does not include three passenger transport modes present in ICCT: buses, civil aviation, and rail transport. In the ODYM-COPPER model, these sectors are included but only for copper assessment, meaning additional material content data must be collected and incorporated. Moreover, as specified in KLOSE and PAULIUK (2023), the fleet demand projection for these modes is simplified, adopting a linear growth factor proportional to GDP growth. This approach seems limited given the potential for passenger transport optimizations aimed at reducing GHG emissions. Thus, although data such as the average lifespan of the existing fleet, probability distribution parameters for fleet lifespan, and material content can be used, the approach should be revised. Since the ICCT model includes emission reduction scenarios and provides fleet data, these data should be utilized.

For the bus mode, ICCT provides fleet data for ICEG, ICED, ICE GNV, and battery electric vehicles; modifications have been made to include ICEE in COFFEE. From the perspective of material demand and lifespan parameters, all ICE bus technologies can share the same parameters, unlike electric buses, which are partially covered in ODYM-COPPER. Data from ODYM-COPPER can be utilized, requiring only the harmonization of the initial existing fleet.

For the aviation mode, again, ODYM-COPPER already includes data on material intensity, the lifespan of the existing fleet, and lifespan distribution parameters, which can be leveraged. The initial year fleet should be harmonized, and future projections should be based on ICCT data.

For the rail transport mode, there is greater complexity, as the infrastructure for this mode can be shared between passenger and freight transport, including both railways and locomotives. A further discussion is made ahead.

A second integration approach considers that the ICCT model has been discontinued and requires updates regarding constants such as vehicle occupancy and average mileage traveled. As an example illustrating this shortcoming, at the time of its creation in 2012, passenger transport applications were not yet a consolidated reality. However, it is understood that the Gompertz curves on which the model is based can be retained as a method for projecting future transport service demand.

Thus, the ICCT model could provide future transport service demand data to COFFEE, which would carry out the current optimization process, including providing the shares of technologies within a specific transport modal. Meanwhile, fleet construction and material demand calculation would use the same vehicle occupancy and mileage data currently employed by ODYM-RECC. In this case, the fleet calculation step would be retained but would require recalibration of the model to ensure that the projected fleet for the base year is consistent with the existing fleet data. This approach would allow the reproduction of the ME strategies originally envisioned in ODYM-RECC.

For the input data, the values for energy services would need to be replaced in the calculation spreadsheets with those provided by COFFEE along with the technological distributions. Harmonization with these distributions within the file `3_SHA_TypeSplit_Vehicles_V3.0` will be required, as well as with the regions.

Finally, except for the macroeconomic data, all other inputs would remain unchanged.

A third, more comprehensive and complex approach would involve expanding the scope of the HERMES model (Historical Trends For Mobility Assessment), developed as a result of the doctoral thesis by CALLEGARI (2021). The work was motivated by some criticisms directed at IAMs. The main critique is that IAMs focus heavily on the supply-side, seeking to meet energy demand with sources that best adapt to the constraints of imposed scenarios, but without considering potential changes in the demand profile, which is typically constructed in an aggregated form with few factors representing the narratives of these scenarios. Another issue is that the passenger transport sector is highly influenced by behavioral factors. A simple example cited in the thesis is that if least-cost fulfillment were the primary factor of choice, most people would opt for public transport or, in the case of private transport, for economy cars.

The model is thus designed to calculate passenger transport service demand and modal share by considering the following aspects:

- Calculation of demand in pkm, which can be interchanged between modes;
- Travel time and speed, as well as user preferences for both;
- National income levels;
- Ability to address shocks, such as COVID-19;
- Carryover effects of modal demand from the previous period;
- Impacts of the shadow economy.

The model is currently built for four regions: USA, EU, Brazil, and Japan. It could be expanded to the other 14 regions of COFFEE and serve as a satellite model in soft-link with COFFEE. Even in this approach, ODYM-RECC would receive transport service data with the modal shares but without further subdivision within each mode (e.g., electric cars vs. ICE vehicles), and the same harmonization proposed for the second approach would be applied here.

4.3.1.2 Freight Transportation

The freight transport sector is not included in ODYM-RECC but is partially described in ODYM-COPPER, albeit not with the same resolution as ICCT or COFFEE. For this sector, COFFEE can provides the transport service profile (tkm) served by each mode for each region.

Unlike passenger transport, this sector is less subject to changes in demand profile due to consumer preferences and, in practice, tends to follow a least-cost strategy for meeting demand. As another difference compared to passenger transport, where different occupancy rates and mileage per period are estimated to determine fleet size, for freight transport, typical tkm activities per modal unit are estimated (GHISOLFI *et al.*, 2024), which can be used to estimate the fleet size for each mode. Formula 4.2, where m is the index for the modal type, shows the calculation.

$$(\text{fleet})_m = \frac{(\text{transport service})_m}{(\text{transport activity/vehicle})_m} \tag{4.2}$$

For trucks, the ODYM-COPPER database should include greater detail for truck classifications. The topologies covered by ICCT are LHDT (Light Duty Truck), MHDT (Medium Duty Truck), and HHDT (Heavy Duty Truck). It is understood that at least the material intensity should be differentiated, while retaining the lifespan values of the existing fleet and the parameters of its distribution.

In an initial approach, the vessel fleet will continue to be described as a typical 1500-tonne vessel, as per SCHIPPER *et al.* (2018), based on data from EQUASIS (2014). These data may eventually be updated to reflect the most recent publication from 2022 EQUASIS (2022). This publication also provides data on fleet size, lifespan of the current fleet, estimated lifespan for each vessel type, and other details for future subdivision of ship typologies.

It is important to note that, due to the ambitious decarbonization targets for the global shipping fleet set by the International Maritime Organization (IMO) by 2050, new vessel technologies are expected to enter operation, necessitating future enhancements in the description of this mode.

4.3.1.3 Further Discussions on the Transportation Integration

For the road transport sectors of passengers and freight, the ideal approach from the perspective of material demand would also include modeling the infrastructure, given the need for a road infrastructure that is highly intensive in the use of cement, gravel, and asphalt. Again, the new version of ODYM-RECC promises to address this sector, providing a more detailed bottom-up description of demand, especially for the cement sector and non-energy products produced in refineries. Furthermore, VAN ENGELENBURG *et al.* (2024) compiles a rich database that can be used to construct the inputs for ODYM-RECC. For the current integration, this topic will not be addressed. However, if future updates to ODYM-RECC do indeed include it, adaptations for integration will be required.

Another point of note is that some ME strategies used in ODYM-RECC may not be applicable with the first integration approach. Since the fleet is already provided by the ICCT model, strategies like fleet reduction via car sharing or increased annual mileage could not be implemented in ODYM. However, the ICCT model adopts certain emission reduction strategies that also imply a reduction in material use. The following strategies can be found in the model documentation that fits into the case: "transportation activity reduction through travel demand management, land-use policies, and improvements in the efficiency of passenger and freight transportation systems" and "mode shift to less energy-intensive modes (passenger and freight)."

A third important point is the contrast between simulation and optimization. In the ODYM-RECC approach, choices are made regarding different ME narratives, which translate into how fleet occupancy is structured, behavioral options, kilometers traveled per vehicle, vehicle archetypes, and so forth. In the COFFEE approach, a given demand is met at the lowest cost subject to scenario constraints. In this second approach, the choice of a specific fuel type, for example, emerges as a result of the simulation. In any case, COFFEE does not output a vehicle fleet but instead provides the share of the total demand fulfilled by vehicle techs or transport mode (2- or 3-wheelers, cars, buses, trains) and by technology (electric, ICE ethanol, etc.). Ideally, a comprehensive modeling of the transport sector demand within the IAM, allowing for both intermodal and fuel substitutions, would have the greatest potential to reduce energy demand. However, this is the most complex modeling approach and likely the most computationally demanding of those proposed here.

A final consideration pertains to train transportation. Material demand assessment for this mode typically involves analyzing track length and route (or rail) length [2]. By estimating the number of locomotives and compositions per kilometer, the existing material stock can be calculated. Current data on installed capacity is available in INTERNATIONAL UNION OF RAILWAYS (UIC) (2024). For projecting demand growth, S-shaped functions are often employed, as demonstrated by SCHIPPER *et al.* (2018) and KLOSE and PAULIUK (2023), which use the following formula:

$$\begin{aligned}&\text{Track length from the previous year} + (\text{Maximum estimated tracks} - \\ &\qquad \text{Track length from the previous year}) \times \text{Growth factor}\end{aligned} \tag{4.3}$$

However, this approach represents a top-down construction of railway infrastructure demand. The proposed approach aims to translate pkm and tkm demand into infrastructure requirements. While the detailed strategy will not be addressed here, it is understood that the process should involve the following steps:

1. Distinguish the portion of the current railway-specific infrastructure (wagons and locomotives) allocated to passenger and freight services. This could utilize the formulas 4.1 and 4.2 from the previous section with appropriate adjustments.
2. Determine how much of the current track length and route length (fixed in-

[2]The key distinction between track length and route length lies in their measurement: track length refers to the total length of all tracks within a rail network, whereas route length represents the distance covered by railway routes available for train operations.As a result, for example, a double-track route will have a track length that is double the length of its route length.

frastructure) is shared, dedicated to freight only, or allocated exclusively to passenger services.

3. Translate pkm and tkm into segregated specific and fixed infrastructure requirements.
4. Assess the potential for future shared use of track and route lengths. In scenarios such as SSP1 or LEDs, allocate a larger share of routes to mixed-use.

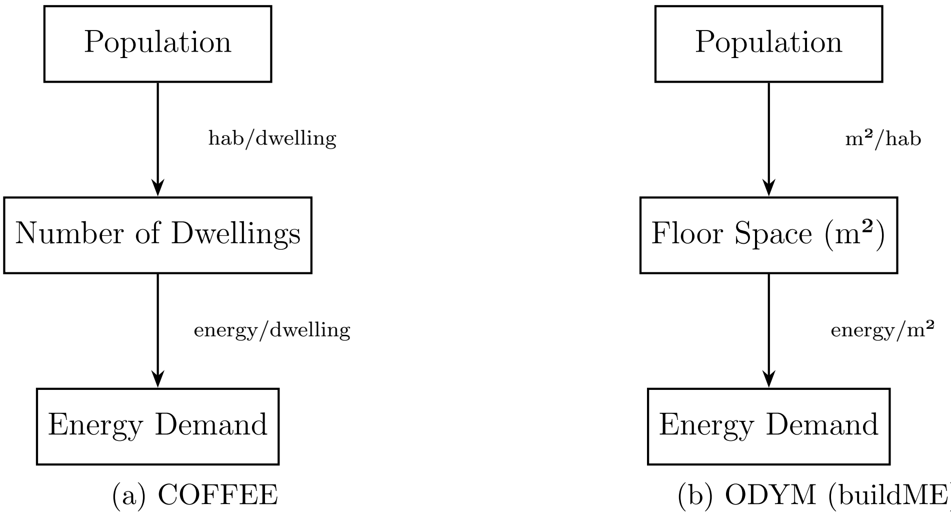
4.3.2 Integration for the Buildings Sector

4.3.2.1 Residential Sector

For the residential sector, the proxies used to determine total energy demand in COFFEE differ from those used in ODYM-RECC (which also uses them to calculate material demand). As previously discussed, COFFEE adopts a sequence shown in Figure 4.1a, leading to a final energy demand subdivided into six categories: space heating, water heating, cooking, appliances, cooling, and lighting.

In COFFEE, there is no detailed description of housing types or more granular energy consumption patterns; data are handled in an aggregated manner, with only the regional subdivision of the IAM itself. For these regions, specific factors for inhabitants per dwelling and energy demand per dwelling are applied. COFFEE does provide a more detailed description of heating and cooling demands using CDD (Cooling Degree Days) and HDD (Heating Degree Days) factors. It also subdivides lighting demand into electric and non-electric (kerosene, paraffin, etc.). Finally, the data on inhabitants per dwelling undergo pre-processing to vary over time based on the GDP per capita of the macroeconomic scenario inputted.

Figure 4.1: Relationships between population and total energy demand for the residential sector



(a) COFFEE (b) ODYM (buildME)

ODYM-RECC makes use of a Python-based software called buildME (HEEREN *et al.*, 2023), which, in turn, uses EnergyPlus (U.S. DEPARTMENT OF ENERGY, 2024) for energy demand calculations. The buildME works with the following aspects: region, occupation, climate region, climate scenario, cooling type, energy standard, and resource efficiency scenario (RES). The first two are embedded in the building archetypes used (discussed later), allowing the occupancy rate per m^2 of dwellings in each region to be specified. The climate region aspect defines the climate characteristics to which the buildings will be subjected and is based on U.S. climate divisions, which are understood to serve as proxies for other regions of the globe. The table with the climate regions, descriptions, proxy cities, HDD, and CDD is presented in Table 4.22.

The "climate scenario" aspect allows the choice of the simulation's climate scenario, enabling different RCPs to be simulated in the model, resulting in varying energy demands, for example, for cooling. The "cooling" aspect refers to the type of internal temperature control to be adopted, whether conventional HVAC (Heating, Ventilation and Air Conditioning) or MMV (Mixed Mode Ventilation)[3]. The RES aspect was adapted by ODYM-RECC to align with the strategies used there. Finally, the "energy standard" aspect includes four possibilities, which are described in Table 4.23 and are fully utilized in ODYM-RECC.

Table 4.22: Climate Zones (SOURCE: HEEREN *et al.* (2023))

Climate Zone	**Description**	$HDD_{18^\circ C}$	$CDD_{10^\circ C}$	**Representative City**
0	Extremely hot	n/a	6000 < CDD	
1A	Very Hot – Humid	n/a	5000 < CDD	Miami, Florida
1B	Very Hot – Dry	n/a	5000 < CDD	Apparently not found in US
2A	Hot – Humid	n/a	3500 < CDD ≤ 5000	Houston, Texas
2B	Hot – Dry	n/a	3500 < CDD ≤ 5000	Phoenix, Arizona
3A	Warm – Humid	n/a	2500 < CDD ≤ 3500	Atlanta, Georgia
3B-Coast	Warm – Dry	n/a	2500 < CDD ≤ 3500	Los Angeles, California
3B	Warm – Dry	n/a	2500 < CDD ≤ 3500	Las Vegas, Nevada
3C	Warm – Marine	HDD ≤ 2000	CDD ≤ 2500	San Francisco, California
4A	Mixed – Humid	2000 < HDD ≤ 3000	2500 < CDD	Baltimore, Maryland
4B	Mixed – Dry	2000 < HDD ≤ 3000	2500 < CDD	Albuquerque, New Mexico
4C	Mixed – Marine	2000 < HDD ≤ 3000	n/a	Seattle, Washington
5A	Cool – Humid	3000 < HDD ≤ 4000	n/a	Chicago, Illinois
5B	Cool – Dry	3000 < HDD ≤ 4000	n/a	Boulder, Colorado
6A	Cold – Humid	4000 < HDD ≤ 5000	n/a	Minneapolis, Minnesota
6B	Cold – Dry	4000 < HDD ≤ 5000	n/a	Helena, Montana
7	Very cold	5000 < HDD ≤ 7000	n/a	Duluth, Minnesota
8	Subarctic	7000 < HDD	n/a	Fairbanks, Alaska

It is important to note that buildME allows for a greater variety of building archetypes, including the possibility for users to create new ones. The official documentation provides examples of some native archetypes and others created for aca-

[3]More on this mode can be found in `https://github.com/NTNU-IndEcol/BuildME/blob/master/docs/afn-mmv.md`

demic studies. ODYM-RECC utilizes the residential archetypes of SFH (Single Family House), MFH (Multi Family House), and RT (Residential Tower) and combines some non-residential archetypes to form the six used in ODYM for Non-Residential. Furthermore, as previously discussed, each archetype can also have constructive variations in energy standards as outlined in Table 4.23. These archetypes, along with the climate regions and climate scenarios files, are input into the thermodynamic energy model EnergyPlus in the form of .idf and .epw files. EnergyPlus is a free software developed with funding from the U.S. Department of Energy (DoE) and is described on its website `https://energyplus.net/` as: "EnergyPlus™ is a whole building energy simulation program that engineers, architects, and researchers use to model both energy consumption—for heating, cooling, ventilation, lighting and plug and process loads—and water use in buildings." The model works with Building Energy Modelling (BEM), which is defined in its documentation (U.S. DEPARTMENT OF ENERGY, 2024) as:

> "Building Energy Modeling (BEM) is the practice of using computer-based simulation software to perform a detailed analysis of a building's energy use and energy-using systems. The simulation software works by enacting a mathematical model that provides an approximate representation of the building. BEM includes whole-building simulation as well as detailed component analysis utilizing specialized software tools that address specific concerns, such as moisture transfer through building materials, daylighting, indoor air quality, natural ventilation, and occupant comfort. BEM offers an alternative approach that encourages customized, integrated design solutions, which offer deeper savings. Using BEM to compare energy-efficiency options directs design decisions prior to construction. It also guides existing building projects to optimize operation or explore retrofit opportunities."

Table 4.23: Energy Standards in buildME (SOURCE: HEEREN *et al.* (2023))

Energy Standard	**Conductivity λ**	**Thickness d**	**Transmittance U**	**Airtightness Standard**
Non-standard	0.10	0.02	2.70	Poor
Standard	0.04	0.12	0.33	Medium
Efficient	0.04	0.16	0.24	Good
ZEB	0.04	0.20	0.19	Excellent

The EnergyPlus model, called by buildME during its execution for energy demand calculation, provides the following energy consumption outputs:

- Cooling:EnergyTransfer (kWh)
- Heating:EnergyTransfer (kWh)
- InteriorEquipment:Electricity (kWh)
- InteriorLights:Electricity (kWh)

The four outputs are compatible with four of the six inputs used by COFFEE, derived from the IEA database, with only cooking and water heating demands missing. According to the EnergyPlus documentation, given the possibility of integrating space heating and cooling systems with water heating systems, the software covers both consumptions in an integrated manner. Therefore, to fully address the residential energy consumption typologies in COFFEE, only the cooking demand, which is not handled by EnergyPlus/buildME, would need to be added. For cooking energy, although the pre-processed data used for COFFEE employs energy per dwelling as a metric, the same IEA database provides data in terms of energy per built area or as a percentage of the total (IEA, 2023).

Thus, there are two main possibilities for integrating this sector. The first is that the residential energy demand inputted into COFFEE is supplied by a prior run of ODYM-RECC or even buildME separately (the logic for the sequence of runs, data feeding, and feedback will be discussed in a later section). This strategy would increase the granularity of the sector in COFFEE without requiring changes to its core. It is worth noting that EnergyPlus allows the creation of new residential archetypes, modeling new climate regions, among other capabilities, which could enhance the sector's description in the future using a software dedicated to this function. Another important point to note is that the enhancements made to COFFEE regarding lighting demand, that is, the segregation between electric and non-electric demand, can be utilized, as it is described as a percentage of the total lighting demand.

This approach has the advantage of simplicity, as COFFEE naturally receives a demand vector to be met for this sector, which would continue to be the case, but linked to scenarios where the modeler could make an a priori choice of efficiency scenarios. Despite its apparent simplicity, there is a calibration challenge. This is because the sum and profile of the total buildings for the base year inputted into the system must closely align with reality, and the energy demand calculated by buildME for that year must also be consistent with real-world data.

From the perspective of the data obtained, there is a disadvantage in terms of future outlook: when energy demands derived from pre-established scenarios are inputted, the choice of certain technologies does not involve optimization and is not subject to constraints. This occurs because it is a simulation model, whereas COFFEE is an optimization model. During optimization, the model can make decisions based on lower costs or to meet constraints. For instance, it may choose to replace a poorly insulated building with one that has better thermal insulation rather than opting to meet a heating demand by replacing a less efficient heat pump with a more efficient one.

The other approach would involve replicating the building archetypes already represented in buildME within COFFEE. This approach, depending on the desired level of detail, is challenging to implement for several reasons. The first challenge is the need to create a strategy of options and their associated costs. Some of these options could include: constructing more efficient buildings, replacing buildings with more efficient ones, using more efficient equipment, adopting cleaner or more efficient fuels, among others. The strategy would need to account not only for the cost of each option but also for feasibility rules, such as determining at what point in its lifespan a building would be eligible for replacement.

Another difficulty with this implementation lies in obtaining data about existing installations, such as: the profile of cooling and heating equipment currently installed by region; the average lifespan of installations and buildings (partially available in ODYM-RECC for buildings); current and future costs of each technological option; emission contributions of each technology; and others.

Essentially, modeling the buildings sector within COFFEE would involve not only the buildings themselves but also the energy-consuming equipment (appliances) within them. This would require constructing the sector's energy demand in a bottom-up manner with a detailed description of its components. Despite the complexity of the modeling, in addition to the already mentioned advantage of optimized technology selection, which is less dependent on the modeler's vision, this approach would also open up possibilities for implementing human behavior models. Examples include preferences for houses versus apartments, shared or individual housing, and other personal or public policy-driven choices.

In this alternative, the building archetypes and their quantities would be provided by COFFEE and inputted into buildME/ODYM-RECC, which would use only its materials module to calculate the demand, as described later.

Finally, despite the strategy adopted for the integration, buildME, using its `calculate_material()` model, also analyzes the demand for the following materials:

- Cement
- Concrete
- Construction grade steel
- Glass
- Insulation material
- Paper and cardboard
- Wood and wood products

4.3.2.2 Non-Residential Sector

For the service building sector, COFFEE employs a methodology identical to that of the residential sector but, as discussed in Chapter 2, uses energy demand per m^2 as a proxy and describes the same six types of final energy services. In this sector, there is also no distinction between building types.

ODYM-RECC, on the other hand, follows exactly the same methodology it uses for the residential sector, including the same ”energy standards” used for residential buildings. The difference lies in the archetypes, which are divided as described in the ”non-res buildings” column of Table 4.20.

Given the points mentioned above, the same discussions and possible approaches for the residential sector are applicable to the service buildings sector.

Finally, based on the discussion, all database files in ODYM-RECC related to building parameters will be retained if the first integration option is to be adopted. For this option, it is worth noting that, unlike the transport sector, where ICCT simulates some efficiency scenarios, for the building sector, only the different SSPs cause variations in the sector's final energy demands. Given that the macroeconomic data will be shared between both models, ODYM-RECC can also provide COFFEE with variations in energy demands for the sector under each simulated SSP through the application of some of the RECC-modeled strategies.

4.3.3 Integration for the Infrastructure Sector

4.3.3.1 Integration for the electrical infrastructure sector

For the infrastructure sector, KLOSE and PAULIUK (2023) modeled the sector within ODYM using the methodology described in DEETMAN *et al.* (2021). The methodology starts with the current length of transmission and distribution electrical networks, as well as the number of transformer units and substations in each of the 26 regions of the IMAGE model, listed in Table 4.24. For projecting future demand, it assumes that the proportion between the installed electric generation capacity and the dimensions of these networks will remain constant. Additionally, it adopts certain assumptions to quantify the demand for ancillary energy storage structures, considering the increasing deployment of intermittent generation. Thus, the model begins with an estimate of the current length of high-, medium-, and low-voltage grids, as well as associated substations and transformers. For each new delta of installed generation given by IMAGE results, new associated infrastructure is added following specific proportionality rules.

Using material intensity factors from the literature for the listed equipment, including electric generation, the model simulates the stock and demand for the following materials: iron, steel, copper, aluminum, lead, and glass. It is important to note that the model accounts for a variety of network types, not only by the voltage levels mentioned but also by line types (AC and DC), as well as whether the lines are underground or overhead.

Table 4.24: Regions in the infrastructure sector

Brazil	India	Oceania	USA
Canada	Indonesia	Russia	Western Africa
Central America	Japan	South Africa	Western Europe
Central Asia	Korea	South Eastern Asia	Rest of South America
Central Europe	Mexico	Turkey	Rest of South Asia
China	Middle East	Ukraine	Rest of Southern Africa
Eastern Africa	Northern Africa		

For this sector, COFFEE outputs on the increase in installed generation capacity at each time interval would be used as direct inputs to ODYM-RECC, similar to how IMAGE outputs were used in ODYM-COPPER. Additionally, regional harmonization is required. Since the initial parameters are the sums of network lengths and the quantities of transformers and substations, this is not a complex task. A similar proposition was made in a collaboration by the present author in work submitted to the 2021 annual IAMC conference [4]. In that case, the aggregation was greater, working with only five regions. For the situation described here, harmonization of the table 4.25 is proposed.

Table 4.25: Mapping of Regions between COFFEE and IMAGE Models

COFFEE	**IMAGE**
Africa (except South Africa)	Northern + Eastern + Western + Rest of southern Africa
Australia and New Zealand	Oceania
Brazil	Brazil
Central America	Central America + Mexico
Canada	Canada
Caspian Region	Central Asia
China	China
East European (EU)	Central Europe + Ukraine + Turkey
India	India
Japan	Japan
South Korea	Korea
Middle East	Middle East
Rest of Asia and Oceania	Indonesia + South Eastern Asia + Rest of South Asia
Russia	Russia
South Africa	South Africa
South America (except Brazil)	Rest of SA
United States	USA
West Europe	Western Europe

4.3.3.2 Integration for other infrastructure sectors

Although there is an intention to model the road and rail infrastructure sectors, they are still in the preliminary stages. The sector was partially modeled in

[4]Link to the poster presented at `https://qiqochat.com/a/dAdDmCWzivyAfPLvKnXaVYWfmURkmNQ`

ODYM-COPPER, but only for copper demand in electrical installations. Some relationships necessary for describing the sector are not yet well defined, even in ODYM-COPPER. Examples of such relationships include those linking, for instance, the size of the vehicle fleet with the extent of the network, or transport service with network length. Other possible relationships might involve population, income, GDP, and country area; for example, a more developed country tends to have a denser road network. Thus, due to its lack of maturity, this sector will not be addressed here.

4.3.4 Integration Diagram

The diagram in Figure 4.2 illustrates the proposed integration. It is important to note that the integration has not yet been implemented, so none of the items are currently functional. However, the distinction between "implemented" and "to be implemented" pertains to features of each model that currently either allow or do not allow integration. Based on the discussion above, the definitive proposal and the information flows will be addressed in the following sections using the diagram as an illustration.

4.3.4.1 Transportation Sector

As previously discussed, there are different proposals for this integration. The one that seems most feasible at this stage and addresses the issue of outdated data in the ICCT model is for it to be responsible for the dimensioning of transport service demand, for both freight and passengers. COFFEE will absorb the service demand in pkm and tkm and the division by vehicle technologies. Internally, it will convert this into secondary and primary energy to optimize costs in the energy sector. ODYM-RECC will receive the demand for these services and return the fleet and the material demand required to meet it.

This approach is expected to harmonize the fleet used by both models, ensure minimal data manipulation, and enable the ME options of ODYM-RECC.

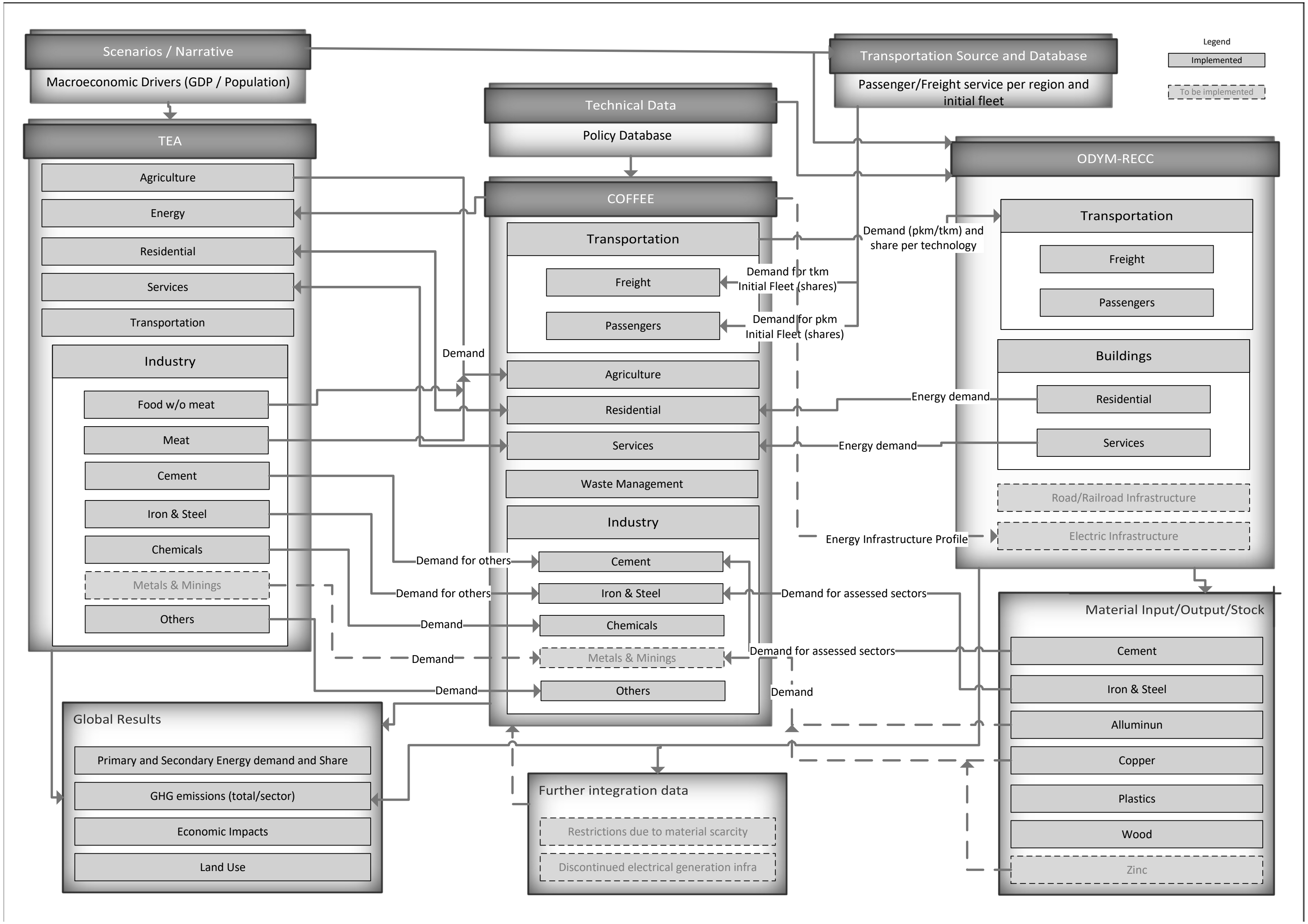


Figure 4.2: Diagram of the proposed integration

4.3.4.2 Buildings Sector

In the previous section, a discussion of the possible approaches for this sector was presented. Aiming to provide indications for future work, which will be addressed later, it is understood that the first option is the most viable when the objective is to focus on the materials model. The second option, which involves enhancing the buildings sector within COFFEE, would require a specific effort for its implementation, potentially covered in a master's dissertation or doctoral thesis.

For the buildings sector, the proposed integration involves a preliminary run in ODYM-RECC, which will provide both the material demand and energy service demand for the sector. This strategy considers that the buildings sector in COFFEE is still underdeveloped. The existence of a fully implemented model with a rich representation of various building archetypes and the fact that COFFEE currently only receives service demand inputs to be met with its modeled primary and secondary energy sources make this integration both feasible and desirable, enhancing COFFEE's scope for the buildings sector avoiding the effort and complexity of modeling the sector within the IAM.

4.3.4.3 Electrical Infrastructure

For the infrastructure sector, the methodology used in (DEETMAN *et al.*, 2021) and in (KLOSE and PAULIUK, 2023) assumes that the system receives the input of the electricity generation profile for the scenario before assessing material demand. Thus, for a complete run of ODYM-RECC, a COFFEE run is required to provide these inputs.

Although at a more advanced implementation stage than road and rail infrastructure, given that it has already been implemented in a separate ODYM model to evaluate the copper cycle, the electrical infrastructure sector has not yet been integrated into ODYM-RECC and has been included in the diagram as a future implementation. As will be discussed in the following section, this sector could play an important role in closing economic cycles linked to materials, such as a potential increase in the installation cost of certain generation technologies depending on their reliance on, for example, critical materials.

4.3.4.4 Industrial Sector

The proposed integration between the IAM and the dMFA model will enable the bottom-up calculation of material demand. As previously discussed, this demand is usually generated by the CGE model or another macroeconomic model in a top-down manner, typically relying on relationships with macroeconomic drivers for an aggregated total demand. The proposed integration will allow the demand to be disaggregated and constructed by sectors. In this situation, the total demand can only be accurately represented if all demand sectors are modeled, which is not currently the case. To address this issue, a similar approach to that used for the chemicals sector by ZOTIN (2024) is proposed, where the most representative slices are described, and the remainder is aggregated into a generic category called "others." This methodology, the third option listed in 3.3.6, provides a detailed bottom-up construction for the most representative sectors of a given material's demand (e.g., buildings and infrastructure for cement) and a top-down approach for the rest.

To implement this strategy, it is crucial to have data on the current demand for the evaluated materials divided by sector. The shares of the modeled sectors would be excluded from the macroeconomic projection currently provided by the CGE, which would only project the demand for "others." As shown in the diagram, for demands such as iron and cement, part of the demand would be supplied by ODYM-RECC and the other part by the CGE.

This approach, while more costly in terms of pre-configuring the models, offers several advantages. The first is the ability to capture changes in the demand profile for certain materials in decarbonization scenarios; for example, the steel sector might experience increased demand in such scenarios, which cannot currently be captured using an aggregated top-down demand approach that tends to reproduce past behavior into the future. The second is the possibility of modular sector construction. Once the methodology is established, it becomes necessary only to remove the modeled sector's share from the CGE's aggregated sector demand to incorporate the bottom-up modeling in ODYM-RECC. For instance, the infrastructure sector for roads in ODYM-RECC is not yet fully modeled, nor is its demand for steel and cement. However, once implemented, segregating the demand for these materials from the aggregated demand provided by the CGE to absorb the bottom-up modeling becomes more straightforward.

4.3.5 Integration Loops and Run Sequence

This section will address the sequence of operations and the feedback loops between the models based on the integration options discussed in the previous section. For the transport sector, it will be necessary to run COFFEE first, as the split between archetypes within each mode will be partially provided by it. As previously mentioned, for the buildings sector, an independent run of buildME, separate from ODYM-RECC, is proposed. This run, lighter than a full ODYM-RECC run, will provide energy demand vectors for the sector to COFFEE's first run. The material function run of buildME will supply the primary material demand inputs for ODYM-RECC. For the electrical infrastructure sector, a COFFEE run will also be necessary, which will then provide ODYM-RECC with the initial installed stock and the deltas of entries and exits of installed capacity over time intervals.

For constructing the industrial sector demand, a precedence issue arises: COFFEE must run first to feed ODYM-RECC, but the material demand of the industrial sector (later transformed into energy demand depending on the technological route used) is provided by ODYM-RECC. For this situation, it is proposed to run COFFEE initially with macroeconomic inputs, as is currently done. The output would feed the first complete run of ODYM-RECC, which would then provide material demand data. After convergence, discussed below, the material demand vector obtained from the sequence of iterations could be saved and used as an initial vector in new COFFEE runs for similar scenarios (e.g., SSP2 with a specific carbon budget). As mentioned earlier, ODYM-RECC can capture changes in the profile of a particular type of material that may differ from a purely economic projection. It is essential to analyze these divergences from the perspective of feasibility or even as an indication of a feasible scenario not predicted in conventional modeling.

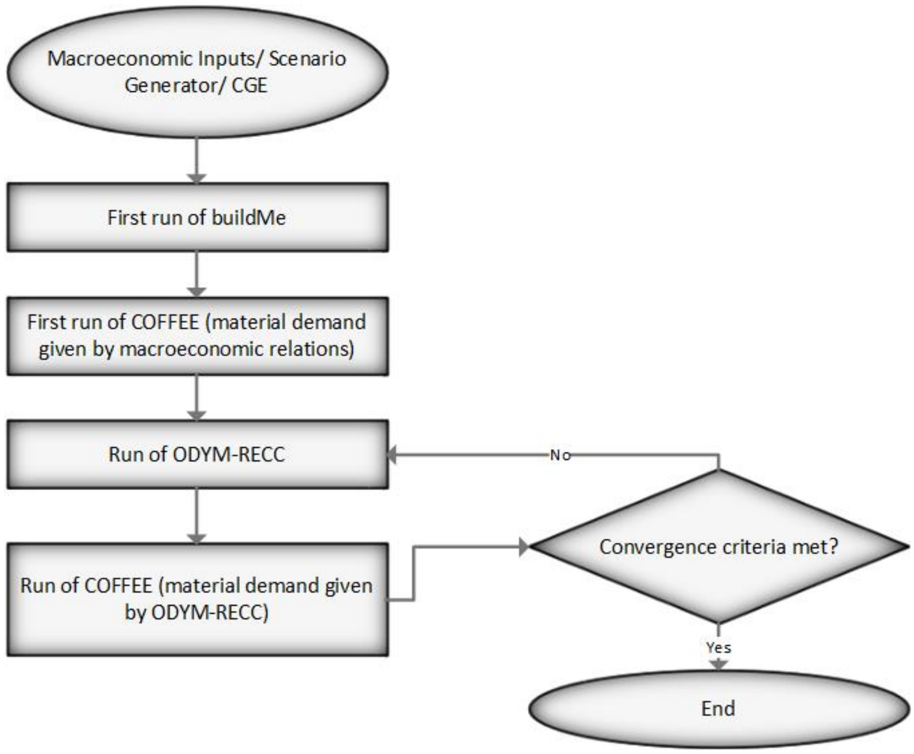


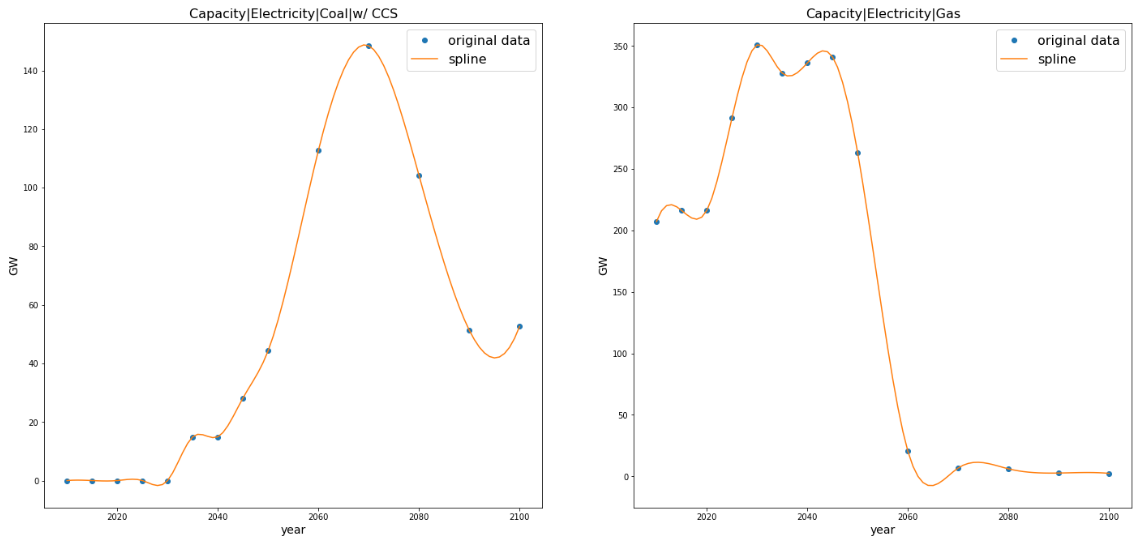
Figure 4.3: Run sequence and loops

A fundamental point is to establish a convergence criterion. From the experience of integrating CGE models with energy models, it is known that convergence across all sectors is not always feasible or may require a large number of iterations (KROOK-RIEKKOLA *et al.*, 2017), (NISHIURA *et al.*, 2024). KROOK-RIEKKOLA *et al.* (2017) established a convergence criterion based on limiting the variation in results between consecutive runs, such as steel inputs, energy demand for the industrial sector, among many others, from one iteration to the next. From an exploratory perspective, analyzing a wide range of variables is essential to investigate potential inconsistencies in model integration. However, after the integration is consolidated, requiring calibration and data adjustments, a simplified strategy could be adopted by selecting a few key aggregated variables as the convergence criterion. The Figure 4.3 illustrates the proposed run sequence and convergence loop.

4.3.6 Time Resolution Harmonization

The third script available in II performs a graphical check of the interpolated data using the first script. It selects the original file and, from this data, creates points that are added along the curve generated by the interpolation. The sample-based check aims to verify: whether the original points are indeed maintained on the resulting curve, whether extreme peaks are not generated, whether oscillations are actually smooth, and whether there are no discontinuities. In figure 4.4 there are some charts obtained from COFFEE outputs.

Figure 4.4: Interpolation test using cubic spline interpolation



There is a potential issue with the proposed interpolation method, namely small overshoots above and below the provided data points. In certain scenarios, these overshoots are considered inappropriate. For instance, in the second image of 4.4, gas generation capacity begins a rapid deceleration from 2045, dropping sharply until 2070 and then following a pattern of gradual decline. It seems unrealistic that, within a market perspective involving such a steep decline, there would be an increase in generation during the 2070–2080 decade, as suggested by the proposed interpolation.

Thus, new interpolation methods were explored, and their advantages or application recommendations can be briefly summarized below (RABBATH and COR-

RIVEAU, 2019): The PCHIP (Piecewise Cubic Hermite Interpolating Polynomial) is an alternative to cubic splines that preserves the monotonicity of the data. This ensures that there will be no overshoots between the given points and is particularly suitable when the data exhibit a clear trend. Another option is linear interpolation, which provides a simple solution that avoids overshoots entirely if smoothness is not essential.

Akima interpolation was also tested; however, it does not guarantee the absence of overshoots. While it produces a smoother curve than cubic splines, it does not offer additional benefits over cubic splines for the case at hand.

Figure 4.5: Interpolation test using PCHIP interpolation

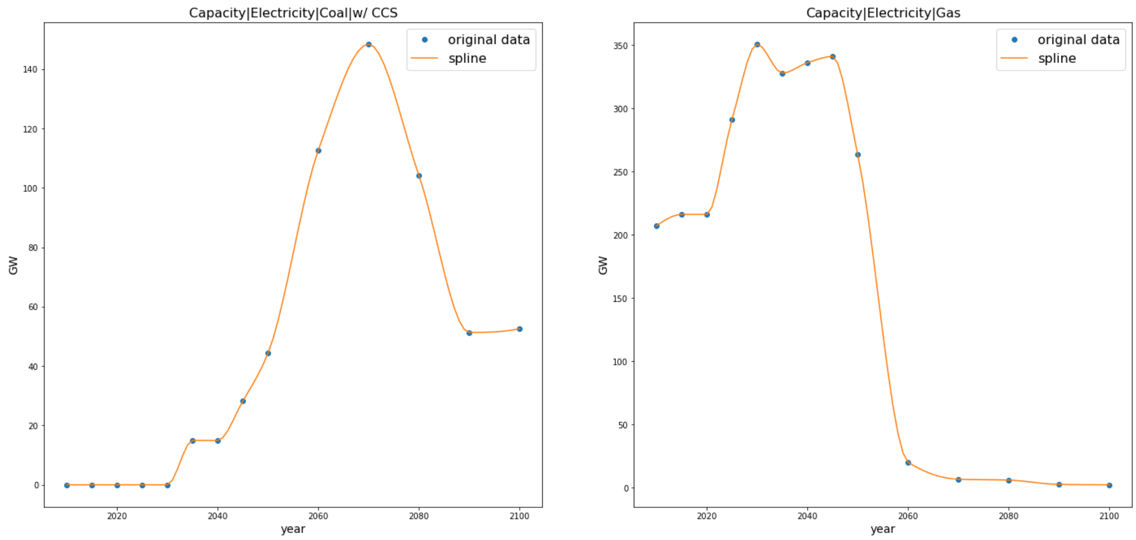
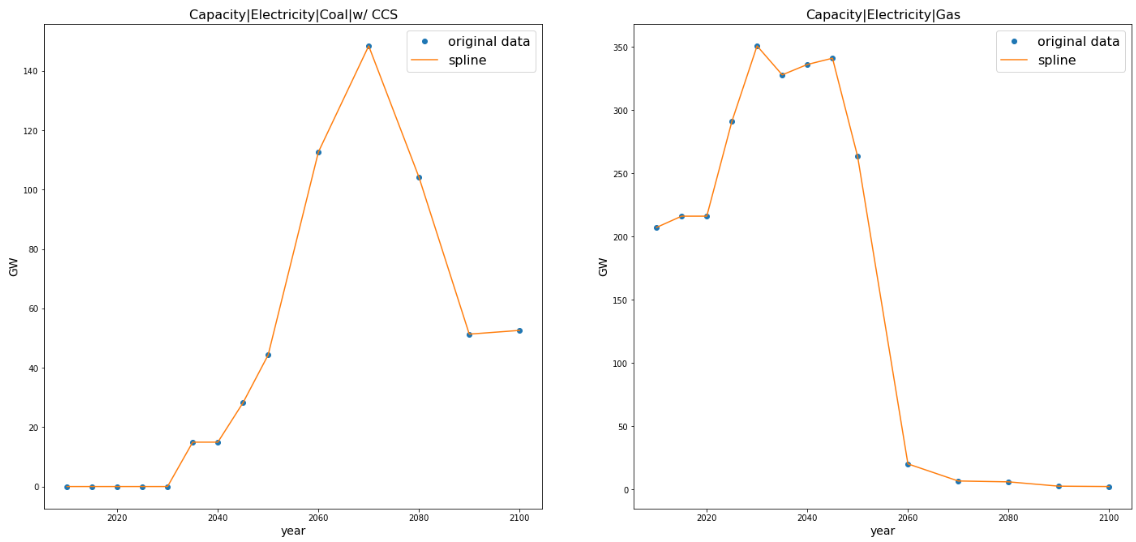


Figure 4.6: Interpolation test using linear interpolation



Figures 4.5 and 4.6 present the same tests for PCHIP and linear interpolation, respectively. The smoothing effect of the first two interpolation methods compared

to the linear method is evident. Moreover, in the images for PCHIP interpolation, it is clear that overshoots have been removed. Based on these findings and the assurance of continuity and adherence to the original data points, PCHIP interpolation is deemed the most suitable method. A new script, based on the first, allowing users to select the type of interpolation, has been added in Appendix II.

Finally, unlike interpolation scripts, which generate new data that may reflect a mathematical method rather than a model narrative, the data extraction script does not require a testing methodology but only verification of correct data extraction.

4.3.7 Region Harmonization

Regional integration must be conducted across at least the four sectors addressed in Section 4.3.4. An interesting advantage of ODYM-RECC is its development in collaboration with the IMAGE team and close ties to the IAM community. Consequently, its regional structure is based on IMAGE or simplifications adopted by the community, such as the division into 5 or 10 regions used in projects like ENGAGE and EDITS. Although ODYM-RECC employs these simplified structures, its database is being developed with the 26 IMAGE regions in mind. A preliminary harmonization proposal was made in Table 4.24, which is already applicable to the electric infrastructure sector.

For the automotive sector, some data, such as vehicle stocks for the 26 regions, are available in ODYM-RECC's database (PAULIUK, 2024). Other data, such as the current and future fleet profiles, are present for some countries not explicitly listed in ODYM-RECC, including Brazil. This database is under construction and would require further development. Necessary data include passenger occupancy, average annual mileage, the share of each vehicle archetype, and more.

For the building sector, a complicating factor is the inclusion of archetypes within buildME. This is a complex task, and a simplified approach that utilizes existing archetypes is preferable. Additionally, an inventory of existing stocks, their distribution by type, and future profile projections must be created. In this regard, the work of MARINOVA *et al.* (2020) provides an important database for the residential sector, divided into the 26 IMAGE regions, with stocks from 1970 to the present and projections through 2050. ZHONG *et al.* (2021) conducts a similar process, including the service sector and extending the analysis to 2060. Both studies were conducted by or in partnership with the ODYM-RECC development team. In both cases, extending the temporal horizon to 2100 and adapting the database to ODYM-RECC's structure would be necessary.

Integration of the industrial sector involves feeding ODYM-RECC's results into COFFEE to construct material demand from a bottom-up perspective. The division of results in the former will mirror that of the input sectors. Thus, once the inputs are harmonized, the outputs will also be harmonized.

4.4 Discussion

4.4.1 Metals Demand and Reserves

A key point to discuss is that ODYM-RECC enables the evaluation of material reserves and resources, particularly metallic ones, allowing for the proper estimation of primary consumption of a given material. If well-modeled, the yields of metal extracted per mass of ore can produce a primary ore demand curve over time. Yields can be described as a function of time, requiring minor adjustments to the software code. This description would enable modeling resource depletion by inputting a trend of decreasing ore grades. Finally, a cost element could also be incorporated through a production cost vector over time.

This approach introduces a narrative of ex-ante costs and depletion that does not account for disruptive events, such as the discovery of a new mineral source. Nonetheless, there are reasonably reliable models of ore concentration reduction, as seen in KUIPERS *et al.* (2018) and NORTHEY *et al.* (2014), which model depletion relationships based on estimated reserves, mass already produced, and other variables.

However, to close the economic loop, it would ideally involve optimizing reserve consumption, which cannot be done within ODYM-RECC due to its nature as a simulation model. Such optimization would require describing reserves and resources in the same way energy resource reserves are modeled in COFFEE: as reserve slots at different price levels consumed over time to meet demand.

One challenge for metals is the scarcity of studies that determine the critical aspects of converting resources into reserves (MUDD and JOWITT, 2018). Additionally, current reserve estimates are often imprecise. For instance, MUDD and JOWITT (2018) highlights that the known amount of copper in deposits is dynamic, as are extraction values. In mineral exploration, many deposits similar to those already exploited are not formally declared, either due to the absence of governmental agencies to do so or because they are held by private or national companies not subject to financial transparency regulations.

Another issue for metals is that their production is often associated with other minerals. For example, only a quarter of silver production comes from silver as the primary product, with the remainder predominantly produced as a co-product or by-product of minerals such as gold, copper, zinc, and lead (ALEXANDER *et al.*, 2019). For cobalt, approximately 94% of its mining is linked to copper and nickel as co-products (ZENG *et al.*, 2022). Thus, there is an interdependence between mineral reserve consumption, and price fluctuations in associated co-products or by-products can render certain deposits economically unviable.

Nonetheless, a simple modeling approach that initially disregards such interdependencies could still provide insights into the sensitivity of extraction price variations. For the issue of reserve declarations, this is less critical for metals included within bulk materials. Such an optimization model would preferably be developed in Python as a satellite model connected via soft-link. The assessment with COFFEE modelers indicates that embedding mineral reserve modeling within the IAM would involve high computational costs for each iteration.

There is another issue regarding mineral assessment, as previously discussed, the model allows for modular construction, and material demand can be built step-by-step. For example, starting with steel, then adding aluminum, and so on, without requiring changes to the software structure. If copper, for instance, has not been included (e.g., data on copper intensity in products, production yields, etc.), its corresponding vector position would simply hold a null value. Thus, the existing model can be adopted and cycles, products, and yields can be added to evaluate, for instance, a specific critical mineral.

4.4.2 Material Cycles

An important feature of ODYM-RECC is the assessment of material flows throughout the entire lifecycle. Some more restrictive decarbonization scenarios are based on assumptions such as high recycling rates and material reuse (CULLEN *et al.*, 2011). However, the path from a material in use to its new use involves several stages with various losses along the way (or recovery yields) (GLÖSER *et al.*, 2013), (CULLEN, 2017), and it demands a different amount of energy compared to obtaining the material from a primary source. Additionally, the material may remain in stock for a certain period and not be readily available for reuse.

ODYM-RECC is designed to naturally track material flows between each stage of the lifecycle, allowing, for instance, the estimation of how much material will be available to re-enter the cycle at each time step. Typically, these assessments are conducted using historical data on the percentage of material demand that can be met through secondary routes. However, this is a dynamic value. If the demand for a material increases over time, it is likely that an increasingly smaller percentage of the total demand can be supplied by secondary sources. Moreover, changes in the residence times of new stocks entering the use phase can also affect the timing of when they will become available again, thereby impacting the percentage of total demand that can be met through non-primary sources.

Another possibility is to create scenarios with higher recycling intensity (improving collection yields, enhancing recovery, reducing losses, etc.) and providing the corresponding energy demand. This capability of the model opens opportunities to explore IAM outputs based on changes in material cycles through *ceteris paribus* simulations—keeping all other variables constant while altering only the yields, to understand how the energy system would be impacted.

To take advantage of this feature, in the proposed integration, material demands must be segregated into primary and secondary demands. These segregated inputs will feed the COFFEE routes, which will assess the corresponding energy demand.

4.4.3 Further Integrations

As shown in the diagram in Figure 4.2, there is the possibility of new integrations, some of which would involve expanding sectors within COFFEE and eventually within the CGE model. One example would be using the demand for timber in construction within the land-use module. A more detailed analysis of how the sector's demand is currently constructed is needed to determine whether this type of demand is already accounted for and, if so, whether it is aggregated or disaggregated.

Another possibility would be the creation of a metals & mining industrial sector as a generator of energy demand within COFFEE. This sector is currently responsible for about 8% of global energy demand (including iron and steel, already described in COFFEE) (RASUL and HERTWICH, 2023). Additionally, it contributes to a range of other environmental impacts such as water consumption (NORTHEY *et al.*, 2016), soil and air toxicity, and others (RASUL and HERTWICH, 2023). From the perspective of broadening the scope of IAM analysis to include environmental impacts estimated by ODYM-RECC, the description of this sector would be highly valuable. The approach to this integration would involve further sectioning the "other industries" category within industrial energy demand.

A third issue not previously addressed is the "Further integration data" box in the diagram in Figure 4.2. Sharp increases in the demand for a specific material could impose constraints on COFFEE. The material demand data obtained from ODYM-RECC would need to be post-processed and could feed COFFEE in two main ways. The first is as a physical constraint, such as a maximum cap on installation—for instance, a limitation on PV panel installations due to a shortage of silver. The second is via price, where a significant increase in the final product's cost makes it less competitive compared to other technologies. In practice, the first could be represented by the second. This could be achieved through the module proposed in Section 4.4.1.

Finally, ODYM-RECC could provide a better profile of the discontinuity in power generation infrastructure. In this case, it is understood that a convergence loop would be unnecessary; the data would merely serve to improve the description of the end-of-life data for installations in a process of comparison and revision of pre-inserted data into COFFEE.

4.4.4 Gaps in IAMs enhanced by the Integration

One of the initial proposals of this work was to evaluate which gaps in IAMs could be addressed through integration. Four main possibilities were covered in Section 2.4.3, and it is understood that all four are adequately addressed in a future integration. The issue of transparency was already discussed in the aforementioned section and is inherent to the design of ODYM-RECC. Additionally, performing the integration requires an understanding of how the IAM being integrated functions, including its inputs, outputs, data processing methodologies, and assumptions. Thus, a comprehensive diagnostic of COFFEE's structure had to be carried out in this chapter. This diagnostic not only outlines the original construction of the IAM but also compiles the improvements made to it over time.

Regarding the second point—improving the representation of material cycles and the link between stocks and services—it is also considered to be addressed. The construction of the vehicle fleet stock for freight and passenger transport, for instance, is a clear example of this link. The material demand for construction linked to the energy service for providing thermal comfort is another. Material cycles were recently discussed in Sections 4.4.2 and 4.4.1. The provision of material demand met by non-primary routes is a clear example, as are the links between energy demand and material demand.

Regarding feasibility analyses, Section 4.4.1 discusses this aspect. Integration introduces a tool for addressing these issues, whether related to reserve availability or increasing production costs. The discussion in Section 4.4.2 also addresses this topic by analyzing the feasibility of meeting material demand through secondary routes, such as recycling end-of-life (EoL) products and primary scrap recycling.

Finally, concerning feedback with IAMs and CGEs, the entire integration proposal is permeated by this premise. The chosen alternative was to create a feedback loop between the systems, particularly between the IAM and the dMFA model, given that little was discussed about CGE integration apart from the industrial sector demand formation. This premise precisely creates the need to discuss integration loops, iteration sequences, and convergence criteria, as addressed in Section 4.3.5. Throughout this work, feedback is discussed both in its constructive form and in terms of the opportunities for investigation and improved results it can provide.

5 Conclusions

The work introduced a method for material assessment, presenting a structured compilation of the theory behind it, its applications, limitations, and how it can enhance the field of integrated modeling. Additionally, there has been a longstanding demand in the IAM community, including at CENERGIA, to address this sector. To meet this demand, the work presented an alternative using software already applied in IPCC publications and in the mentioned community, along with its description, reference materials, and an understanding of its database and functionality. It is worth emphasizing that, given its open-source construction and free-access database, the software can contribute to the development of collaborative research efforts with other research groups.

From a research contribution perspective, this work provided an extensive diagnosis of COFFEE, compiling dispersed data from various studies, which can serve as a reference for consultation and as a source of ideas for future research at CENERGIA. As described in part of the critique in Chapter 2, there is a demand from the scientific community for greater transparency in these models. In this sense, both the description in Chapter 2 and, more specifically, the one structured in Section 4.1 contribute to addressing this need.

From the perspective of integrating a materials model with an IAM, this work presents a discussion applicable to the integration of two generic models of this type, not solely limited to the ODYM-RECC and COFFEE integration. In this sense, it provides a sectoral approach to the input and output data flows for soft-link communication and the IAM gaps that can be addressed through such integration. It also examines the lack of certain data and proposes ways to address this issue.

From a specific perspective, concerning the harmonization of COFFEE with ODYM-RECC, this work uses the diagnosis of both structures to propose concrete approaches for each sector. By discussing the advantages and disadvantages and considering the limitations of this integration within the context of CENERGIA. The section presenting the diagram makes a selection among these proposals for future work, which could be developed in a subsequent doctoral thesis. The chosen approaches are not necessarily the best modeling solutions but are those that fit within the scope of an individual research project. Nonetheless, other more complex solutions, which could be developed through collective efforts, are also suggested.

Additionally, this work also discusses sectors within COFFEE that are currently modeled in a simplified manner. The proposed improvements could lead to new academic studies independent of the integration of a materials model but, if applied, would enhance its potential.

5.1 Limitations and future work

A first limitation of this study is a lack of methodology for editing input and output data, except for temporal resolution. Due to the structure of the ODYM-RECC database, it may be necessary to create scripts for each type of data set (e.g., material intensities, yields, historical fleet, etc.). This type of development is proposed for a future doctoral thesis, which would address the execution of the integration and the running of case studies.

Another limitation lies in the proposed integration of the industrial sector. Dividing the demand for a given material by sectors (e.g., cement for buildings, infrastructure, etc.) assumes the existence of such historical data, which has not been demonstrated. Indeed, for cement, there is a well-known difficulty in obtaining sectoral demand data. This limitation may eventually require a different type of integration than the bottom-up construction of the industrial sector.

Additionally, one of the initial intentions of this work, at the time of its conception, was to address the topic of resource limitations. However, this aspect was minimally explored here. In the discussion section of the previous chapter, a suggestion was made to approach the issue through a satellite optimization model that would address the tracking and consumption of mineral reserves following the same logic as energy resource reserves in COFFEE. Nevertheless, only an initial assessment was conducted on data availability, the platform on which the system would be built, which materials would be initially addressed, how to structure it to be scalable to other materials, and how it would communicate with COFFEE and ODYM-RECC.

Finally and more important, although the integration has not yet been executed and no case studies have been conducted, this work provides an extensive understanding of what needs to be done to achieve this, paving the way for a future doctoral thesis that could focus more on running the integration and obtaining results for scientific production.

In this context, several research ideas emerge. The first would involve assessing environmental impacts such as water usage in more restrictive decarbonization scenarios. This could be achieved by cross-referencing georeferenced water stress indices with the locations of the most exploited deposits in these scenarios.

Another line of inquiry would explore how increases in recycling yields for certain materials, where the secondary route is more energy-intensive, could impact global energy demand and, consequently, associated emissions.

An additional opportunity would focus on assessing the feasibility of critical material availability for the energy transition in decarbonization scenarios or exploring how such demand could influence the prices of bulk materials in the same scenarios and, in turn, the costs of generation sources.

In summary, integrating a materials model with the powerful and comprehensive toolset of an IAM opens up an entire spectrum of new research possibilities in the field of energy planning.

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I Appendix I - Input for AI training in chatGPT

The following text was provided as instructions for the chat created in ChatGPT 4o:

I am writing a master's dissertation. I will send you the PDF of what has been written so far so that you can understand my issue. The name of the PDF is *Dissertacao-Leandro.pdf.* In the chapters "Introduction" and "Bibliography Review," you will find the context and purpose of the dissertation. In "Methodology," the approach to the problem is described. Much of the intended content is found in the section "Gaps in IAMs Potentially Addressed by Dynamic MFA using ODYM."

Essentially, this involves a proposal for the integration of an Integrated Assessment Model (IAM) developed at COPPE-UFRJ, COFFEE, and its general equilibrium model (CGE), TEA, with a dynamic material flow analysis (dMFA) model, ODYM-RECC. The documentation for COFFEE is mainly found in Pedro Rua Rochedo's doctoral thesis, available in the file *Pedro_Rua_Rodriguez_Rochedo.pdf.* The TEA documentation can be found in the file *TEA.pdf* and in Bruno Cunha's doctoral thesis, available in the file *Bruno_Cunha_DOUTORADO-2019.pdf.* Over time, changes have been made to COFFEE that are not fully documented, but some are recorded at `https://www.iamcdocumentation.eu/Model_Documentation_-_COFFEE-TEA`, which you can refer to if needed. Other characteristics of COFFEE-TEA are described in the file *Keppo_2021_Environ._Res._Lett._16_053006.pdf.*

As for the dMFA model, ODYM-RECC, it is part of a framework whose explanatory PDF will be provided under the name *J of Industrial Ecology - 2019 - Pauliuk - ODYM An open software framework for studying dynamic material systems (1).pdf.* It is an open-source model, and its code is available at `https://github.com/IndEcol/ODYM`. Within this framework, a project was developed to evaluate materials in various future scenarios. The model is typically fed with the Shared Socioeconomic Pathways (SSP) and "communicates" with another IAM, IMAGE. This project is called ODYM-RECC, and its code can be found at `https://github.com/IndEcol/RECC-ODYM` (the main code is also in the file *ODYM_RECC_Main.py*, and all other *ODUM_RECC_xxxx.py* files are extensions that can be called by the main file). The version used will be the most recent, v2.5. The documentation for this project (RECC), created within the ODYM framework, will be provided in the PDF named *IEF_WorkingPaper_01_2023_RECC_Model_-Docu_V2_5_GLOBAL*.

In addition, I will include some scientific publications generated with previous versions of RECC, which served as the foundation for the construction of v2.5 and, in some way, integrate IMAGE with ODYM-RECC, usually using outputs from the former as data inputs and assumptions for the latter.

Part of what will be requested in this chat involves understanding the ODYM-RECC code and proposing methods for its integration with COFFEE. My goal is to provide you with parts of the v2.5 code, written in Python, and have you explain briefly what each part of the code does, along with insights for modifications for a project adapted to COFFEE. Questions may also be asked about the ODYM-RECC code, such as "where are the ODYM-RECC outputs?" and "in which section of the code are the input data read?"

The tables below indicates the material used for the chat's training.

File Name	Description
Dissertacao-Leandro.pdf	Master's dissertation on integrating the COFFEE IAM and ODYM-RECC models
IEF_WorkingPaper_01_-2023_RECC_Model_Docu_-V2_5_GLOBAL.pdf	Documentation of the ODYM-RECC model version 2.5 (PAULIUK, 2023)
Pedro_Rua_Rodriguez_-Rochedo.pdf	Doctoral thesis on developing a global integrated energy model, which includes COFFEE (ROCHEDO, 2016)
TEA.pdf	Documentation of the TEA model, a Computable General Equilibrium (CGE) model used alongside COFFEE (CUNHA *et al.*, 2020)
Bruno_Cunha._DOUTORADO-2019.pdf	Doctoral thesis on the development of a CGE model for climate policy, related to the TEA model (DA CUNHA, 2019)
Keppo_2021_Environ._Res._Lett._16_-053006.pdf	Article on exploring diverse capabilities and gaps in Integrated Assessment Models (IAMs) (KEPPO *et al.*, 2021)
J_of_Industrial_Ecology_2019_Pauliuk.pdf	Article describing ODYM, an open framework for dynamic material systems modeling (PAULIUK and HEEREN, 2020b)
J_of_Industrial_Ecology_2020_Pauliuk.pdf	Article on linking service provision to material cycles using the RECC framework (PAULIUK *et al.*, 2021a)
Deetman2021-Electricity-infra.pdf	Study on the projected material requirements for global electricity infrastructure (DEETMAN *et al.*, 2021)
Deetman2020-Global-material-stocks-residential-services-buildings.pdf	Article on modeling global material stocks and flows for buildings (DEETMAN *et al.*, 2020)
Pauliuk2021-Global-scenarios-resource-emission-savings-ME-res-buildings.pdf	Study on global scenarios of resource and emission savings from material efficiency in buildings and cars (PAULIUK *et al.*, 2021d)

Table I.1: Summary of Files Used in ODYM-RECC Interpreter

File Name	Description
`ODYM_RECC_Main.py`	The main script that controls the ODYM-RECC model simulation, handling the overall model logic and connections to other modules.
`ODYM_RECC_Evaluate_Cascade.py`	Script to evaluate and simulate the material efficiency cascade, running through multiple scenario results.
`ODYM_RECC_Evaluate_Scenarios.py`	Used for evaluating different RECC scenarios, particularly related to resource efficiency and decarbonization.
`ODYM_RECC_Evaluate_Sensitivity.py`	Script for conducting sensitivity analyses within the RECC framework, varying input parameters to analyze their effects on outputs.
`ODYM_RECC_Evaluate_BarPlot_ME_Industry_Demand.py`	Generates bar plots to visualize material efficiency in industry demand across different scenarios.
`ODYM_RECC_Evaluate_GHG_Overview.py`	Provides an overview of greenhouse gas emissions based on different RECC scenarios, summarizing GHG outputs.
`ODYM_RECC_Evaluate_Table_Extract.py`	Extracts tabular data from scenario results for further analysis and reporting.
`ODYM_RECC_ScenarioControl.py`	Script used to manage and control the flow of different scenarios within the RECC model.

Table I.2: Summary of Python Files Used in ODYM-RECC Interpreter

II Appendix II - Time step harmonization codes and test codes

```python
"""
Created on Sat Mar 11 19:18:29 2023

@author: LEANDRO
"""

import csv
import numpy as np
from scipy.interpolate import interp1d
import matplotlib.pyplot as plt
import os
import copy

# insert the directory path
directory = 'C://Users//leand//OneDrive//Documentos//PPE//Engage2.0
    _data//Modelos'
csv_files=[]

#loop over all files in the directory
for filename in os.listdir(directory):
    #check if the file is a csv file
    if filename.endswith('.csv'):
        #add the filename to the list of CSV files
        csv_files.append(filename)

# Define the range of years
# The initial year must be changed according to the initial year of
    the IAM
years = np.arange(2010, 2101)

# iterate between all files in the folder and repeat the same
    script for all files
for i in range(len(csv_files)):

```

```python
    # Set the input and output file names - for the output, the [:-4] remove the file extension .csv
    input_file = directory+'//'+csv_files[i]
    output_file = directory+'//Modelos_Interpolated//'+csv_files[i][:-4]+'-interp.csv'

    # Open the input file and read the data
    with open(input_file, 'r') as f:
        reader = csv.reader(f)
        data = list(reader)

    # test if sequence of years do not follow a 5-years step.
    # Test will find blank spaces in first and last row of data
    # Blank positions of each of tested rows will be stored in blank_positions_1 and
    # blank_positions_2, respectively

    blank_positions1 = []
    for i in range(len(data[1][7:])):
    # find blank positions from the eighth column onwards (needs ajust to your data set)
        if data[1][i+7].isspace() or len(data[1][i+7]) == 0:
        # if it is, add the current position to the blank_positions list
            blank_positions1.append(i+7)

    blank_positions2 = []
    for i in range(len(data[len(data)-1][7:])):
    # find blank positions from the eighth column onwards (needs ajust to your data set)
        if data[1][i+7].isspace() or len(data[1][i+7]) == 0:
        # if it is, add the current position to the blank_positions list
            blank_positions2.append(i+7)

    if blank_positions1 == blank_positions2:

        # deepcopy data if needed
        data_bkp = copy.deepcopy(data)

        # delete blank columns (reversed is used because after a del in a column, the next index will chance and a wrong column will be deleted)
        for i in range(len(data)):
            for j in reversed(blank_positions1):
                del(data[i][j])

```

```
        # Create a numpy array with the original years count
        years_orig = np.array([float(x) for x in data[0][7:]])

        # Create the header for the output file
        header = data[0][:7]
        header.extend(str(y) for y in years)

        # Loop through the data rows and interpolate the columns
        interpolated_data = []
        for row in data[1:]:
            new_row = row[:7]
            old_data = np.array([float(x) for x in row[7:]])
            interp_func = interp1d(years_orig, old_data, kind='cubic', fill_value="extrapolate")
            interpolated_data_row = interp_func(years)
            new_row.extend(str(x) for x in interpolated_data_row)
            interpolated_data.append(new_row)

        # Write the output file
        with open(output_file, 'w', newline='') as f:
            writer = csv.writer(f)
            writer.writerow(header)
            writer.writerows(interpolated_data)

    else:
        print('blank positions between columns does not match')
```

Listing II.1: Python script for interpolation COFFEE output to an one year step

```
import csv
import os

"""
Created on Sun Dec 15 13:29:41 2024
@author: leand
"""

# Path to the folder containing the CSV files
input_directory = 'D://OneDrive//PPE//PC_Trampo//Engage2.0_data//Modelos//Modelos_Interpolated//COFFEE 1.1-Interp.csv'
output_directory = 'D://OneDrive//PPE//PC_Trampo//Engage2.0_data//Modelos//Modelos_Extraidos'

# Create the output folder if it does not exist
os.makedirs(output_directory, exist_ok=True)

# Define the desired years
desired_years = [2015, 2020, 2025, 2030, 2035, 2040, 2045, 2050,
```

```
    2060, 2070, 2080, 2090, 2100]

# Loop through the CSV files in the folder
for filename in os.listdir(input_directory):
    if filename.endswith('.csv'):
        input_file = os.path.join(input_directory, filename)
        output_file = os.path.join(output_directory, f'extracted_{
    filename}')

        # Read the input file
        with open(input_file, 'r') as infile:
            reader = csv.reader(infile)
            data = list(reader)

        # Identify the indices of the columns corresponding to the
    desired years
        header = data[0]
        col_indices = [i for i, year in enumerate(header) if year.
    isdigit() and int(year) in desired_years]

        # Create a new table with the desired columns
        extracted_data = []
        extracted_header = [header[i] for i in col_indices]  #
    Header with years
        extracted_data.append(data[0][:7] + extracted_header)  #
    Add the first 7 columns (fixed data)

        for row in data[1:]:
            selected_columns = [row[i] for i in col_indices]
            extracted_data.append(row[:7] + selected_columns)

        # Write the new CSV file
        with open(output_file, 'w', newline='') as outfile:
            writer = csv.writer(outfile)
            writer.writerows(extracted_data)

        print(f'File processed: {filename}')

print('Extraction completed.')
```

Listing II.2: Python script for extract annualized data from ODYM-RECC to input into COFFEE

```
"""
Created on Sat Mar 11 19:18:29 2023

@author: LEANDRO
```

```python
"""

import csv
import numpy as np
from scipy.interpolate import interp1d
import matplotlib.pyplot as plt
import os
import copy

# insert the directory path
directory = 'C://Users//leand//OneDrive//Documentos//PPE//Engage2.0_data//Modelos'
csv_files=[]

#loop over all files in the directory
for filename in os.listdir(directory):
    #check if the file is a csv file
    if filename.endswith('.csv'):
        #add the filename to the list of CSV files
        csv_files.append(filename)

# Define the range of years
# The initial year must be changed according to the initial year of the IAM
years = np.arange(2010, 2101)

# iterate between all files in the folder and repeat the same script for all files
for i in range(len(csv_files)):

    # Set the input and output file names - for the output, the [:-4] remove the file extension .csv
    input_file = directory+'//'+csv_files[i]
    output_file = directory+'//Modelos_Interpolated//'+csv_files[i][:-4]+'-interp.csv'

    # Open the input file and read the data
    with open(input_file, 'r') as f:
        reader = csv.reader(f)
        data = list(reader)

    # test if sequence of years do not follow a 5-years step.
    # Test will find blank spaces in first and last row of data
    # Blank positions of each of tested rows will be stored in blank_positions_1 and
    # blank_positions_2, respectively

```

```
    blank_positions1 = []
    for i in range(len(data[1][7:])):
    # find blank positions from the eighth column onwards (needs ajust to your data set)
        if data[1][i+7].isspace() or len(data[1][i+7]) == 0:
        # if it is, add the current position to the blank_positions list
            blank_positions1.append(i+7)

    blank_positions2 = []
    for i in range(len(data[len(data)-1][7:])):
    # find blank positions from the eighth column onwards (needs ajust to your data set)
        if data[1][i+7].isspace() or len(data[1][i+7]) == 0:
        # if it is, add the current position to the blank_positions list
            blank_positions2.append(i+7)

    if blank_positions1 == blank_positions2:

        # deepcopy data if needed
        data_bkp = copy.deepcopy(data)

        # delete blank columns (reversed is used because after a del in a column, the next index will chance and a wrong column will be deleted)
        for i in range(len(data)):
            for j in reversed(blank_positions1):
                del(data[i][j])

        # Create a numpy array with the original years count
        years_orig = np.array([float(x) for x in data[0][7:]])

        # Create the header for the output file
        header = data[0][:7]
        header.extend(str(y) for y in years)

        # Loop through the data rows and interpolate the columns
        interpolated_data = []
        for row in data[1:]:
            new_row = row[:7]
            old_data = np.array([float(x) for x in row[7:]])
            interp_func = interp1d(years_orig, old_data, kind='cubic', fill_value="extrapolate")
            interpolated_data_row = interp_func(years)
            new_row.extend(str(x) for x in interpolated_data_row)
            interpolated_data.append(new_row)
```

```
        # Write the output file
        with open(output_file, 'w', newline='') as f:
            writer = csv.writer(f)
            writer.writerow(header)
            writer.writerows(interpolated_data)

    else:
        print('blank positions between columns does not match')
```

Listing II.3: Python script for test the interpolation COFFEE output to an one year step

```
# -*- coding: utf-8 -*-
"""
Created on Sun Dec 15 13:56:50 2024
@author: leand
"""

import csv
import numpy as np
from scipy.interpolate import PchipInterpolator,
    Akima1DInterpolator, interp1d
import matplotlib.pyplot as plt
import os
import copy

# insert the directory path
directory = 'D://OneDrive//PPE//PC_Trampo//Engage2.0_data//Modelos'
csv_files=[]

# Choose interpolation method
interpolation_method = 'pchip'  # Options: 'cubic', 'pchip', 'akima
    ', 'linear'

#loop over all files in the directory
for filename in os.listdir(directory):
    #check if the file is a csv file
    if filename.endswith('.csv'):
        #add the filename to the list of CSV files
        csv_files.append(filename)

# Define the range of years
# The initial year must be changed according to the initial year of
     the IAM
years = np.arange(2010, 2101)

```

```
# iterate between all files in the folder and repeat the same script for all files
for i in range(len(csv_files)):

    # Set the input and output file names - for the output, the [:-4] remove the file extension .csv
    input_file = directory+'//'+csv_files[i]
    output_file = directory+'//Modelos_Interpolated//'+csv_files[i][:-4]+'-interp.csv'

    # Open the input file and read the data
    with open(input_file, 'r') as f:
        reader = csv.reader(f)
        data = list(reader)

    # test if sequence of years do not follow a 5-years step.
    # Test will find blank spaces in first and last row of data
    # Blank positions of each of tested rows will be stored in blank_positions_1 and
    # blank_positions_2, respectively

    blank_positions1 = []
    for i in range(len(data[1][7:])):
    # find blank positions from the eighth column onwards (needs ajust to your data set)
        if data[1][i+7].isspace() or len(data[1][i+7]) == 0:
            # if it is, add the current position to the blank_positions list
                blank_positions1.append(i+7)

    blank_positions2 = []
    for i in range(len(data[len(data)-1][7:])):
    # find blank positions from the eighth column onwards (needs ajust to your data set)
        if data[1][i+7].isspace() or len(data[1][i+7]) == 0:
            # if it is, add the current position to the blank_positions list
                blank_positions2.append(i+7)

    if blank_positions1 == blank_positions2:

        # deepcopy data if needed
        data_bkp = copy.deepcopy(data)

        # delete blank columns (reversed is used because after a del in a column, the next index will chance and a wrong column will be deleted)
```

```python
        for i in range(len(data)):
            for j in reversed(blank_positions1):
                del(data[i][j])

        # Create a numpy array with the original years count
        years_orig = np.array([float(x) for x in data[0][7:]])

        # Create the header for the output file
        header = data[0][:7]
        header.extend(str(y) for y in years)

        # Loop through the data rows and interpolate the columns
        interpolated_data = []
        for row in data[1:]:
            new_row = row[:7]
            old_data = np.array([float(x) for x in row[7:]])
            # Method selection
            if interpolation_method == 'cubic':
                interp_func = interp1d(years_orig, old_data, kind='cubic', fill_value="extrapolate")
            elif interpolation_method == 'pchip':
                interp_func = PchipInterpolator(years_orig, old_data)
            elif interpolation_method == 'akima':
                interp_func = Akima1DInterpolator(years_orig, old_data)
            elif interpolation_method == 'linear':
                interp_func = interp1d(years_orig, old_data, kind='linear', fill_value="extrapolate")
            else:
                raise ValueError("Invalid interpolation method selected")

            interpolated_data_row = interp_func(years)
            new_row.extend(str(x) for x in interpolated_data_row)
            interpolated_data.append(new_row)

        # Write the output file
        with open(output_file, 'w', newline='') as f:
            writer = csv.writer(f)
            writer.writerow(header)
            writer.writerows(interpolated_data)

    else:
        print('blank positions between columns does not match')
```

Listing II.4: Python script for interpolation COFFEE output to an one year step

III Appendix III - Analysis of ODYM inputs and necessary changes - Tables

Table III.1: Dados de entrada ODYM-RECC

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
2_P_RECC_Population_SSP_32R_-V2.3 Historic and future population scenarios.	MtrS	Million	Use same scenario database as CGE-IAM.	Yes	Regions Target Year Years step size Population	Use the same database	The transformation from 32 to 18 regions can be performed either within the ODYM script or by modifying the spreadsheet that serves as the database. A "Regions18" aspect must be added to the IndexTable in ODYM
2_S_RECC_FinalProducts_2015_-passvehicles_V1.4 2015 stock by age-cohort.	tcpr	million units	Use the same scenario database as the IAM.	Depending on the IAM	Regions Target Year Years step size Cars Archetipes Types of techs	Use the same database	Only if IAM assess the in use stock of passenger vehicles. In the case of COFFEE, historical vehicle data and future projections come from the ICCT. The spreadsheet that serves as the ODYM database must contain the output data from the ICCT.
2_S_RECC_FinalProducts_2015_-resbuildings_V1.4 2015 stock by age-cohort.	tcBr	billion m2	None	Depending on the IAM	Regions Target Year Years step size Stock	Use the same database	Only if IAM assess the in use stock of residential buildings
2_S_RECC_FinalProducts_2015_-nonresbuildings_V2.2 2015 stock by age-cohort.	tcNr	million m2	None	Depending on the IAM	Regions Target Year Years step size Stock	Use the same database	Only if IAM assess the in use stock of nonres buildings

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
1_F_Function_Future_V1.4 Transport function (passenger vehicle operation) to be fulfilled by the entire fleet, from 2015 to 2100, for each region. the corresponding section in the 'Transport modeling documentation' (Fishman et al., 2021; Wolfram et al., 2020).	GrtS	inhabitant* m2*yr/yr and passenger-km/yr	None	Partial	Regions Target Year Years step size	0	The dataset only provides data for passenger vehicles vs energy service in pkm/yr. Freight fleet or freight energy service is not provided.
1_F_RECC_FinalProducts_appliances_-V1.0 Future and past inflow in use phase, appliances.	ocSRa	Items/yr	IAM, if applicable	Depending on the IAM	Regions Target Year Years step size Types of applian.		It is not common for IAMs to project the demand for appliances. If they do, they usually project the aggregated energy demand. In this case, it would be more appropriate for the IAM to receive the energy demand for this sector from ODYM.
1_F_RECC_FinalProducts_industry_-V1.0 Future and past inflow in use phase, industrial assets (exogenous).	ISRlc	GW/yr	IAM	Depending on the IAM	Regions Target Year Years step size Types of electric generators	Use de IAM output	Here, "industrial" refers to the installed generation capacity.
2_S_RECC_FinalProducts_nonres-buildings_g_V1.0 Future and past in-use stock scenarios for nonres. Buildings, global resolution.	Nc	m^2/yr	IAM	Depending on the IAM	Regions Target Year Years step size	This dataset came from an IAM run, the aspects in collum V must match.	ODYM can pre-calculate demanded area for buildings or have it as an output from an IAM run, this dataset is one of the later cases, it came from an IMAGE run

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
2_S_RECC_FinalProducts_Future_resbuildings_v2.7 Per capita residential floor space tends to increase with GDP, but varies widely across countries at the same level of GDP, shaped by tradition, urban form, as well as land use and building regulations (International Energy Agency, 2016).	sTGr	buildings: m2 per person	None	Depending on the IAM	Regions Target Year Years step size Archetypes Factors	Use the same m2/capita relation factors	Depending on the integration, if the IAM receives the projection of built area and energy demand, only the three mentioned aspects need to be harmonized. Some IAMs evaluate the total construction area of residential buildings, the calculation methodology must be the same as the type of buildings assessed. This dataset relates m2/cap and vehicle/cap depending on region an scenario, this factors must be the same in IAM and ODYM.
2_S_RECC_FinalProducts_Future_resbuildings_MIUPotential_V1.0 This parameter describes the maximum reduction potential for per-capita floor space.	Gos	%	None	Partial	Regions Target Year Years step size	0	It is a dataset to assess efficient scenarios, not necessarily used

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
2_S_RECC_FinalProducts_Future_-NonResBuildings_v2.4 Per capita non-residential floor space varies widely across countries at the same level of GDP, shaped by tradition, urban form, as well as land use and building regulations (International Energy Agency, 2016). The SSP scenarios don't detail the floor space in their documentation, and we formulate values which are consistent with the SSP storylines.	Grts	buildings: m2 per person	None	Depending on the IAM	Regions Target Year Years step size Archetypes Factors	Use the same m2/capita relation factors	Depending on the integration, if the IAM receives the projection of built area and energy demand, only the three mentioned aspects need to be harmonized. Some IAMs evaluate the total construction area of residential buildings, the calculation methodology must be the same as the type of buildings assessed. This dataset relates m2/cap and vehicle/cap depending on region an scenario, this factors must be the same in IAM and ODYM.
2_S_RECC_FinalProducts_Future_non-resbuildings_MIUPotential_V1.0 This parameter describes the maximum reduction potential for per-capita floor space.	Gos	%	None	Partial	Regions Target Year Years step size		This is a reduction factor that is only applied when running the ME strategies.
3_El_Products_UsePhase_passvehicles_-V1.3 Operational energy demand, all energy carriers together.	cpVnrS	Vehicles: MJ/km	IAM	Yes	Regions Target Year Years step size Archetypes Factors	Use the same m2/capita relation factors	

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
3_El_Products_UsePhase_resbuildings_-V1.4 Operational energy demand, all energy carriers together.	cBVnrS	MJ/m2/yr	None	Partial	Regions Target Year Years step size	See coments	Depending on the integration, if the IAM receives the projection of built area and energy demand, only the three mentioned aspects need to be harmonized.
3_El_Products_UsePhase_nonresbuildings_V1.4 Operational energy demand, all energy carriers together.	cNVnrS	MJ/m2/yr	None	Partial	Regions Target Year Years step size	See coments	Depending on the integration, if the IAM receives the projection of built area and energy demand, only the three mentioned aspects need to be harmonized.
3_IO_Vehicles_UsePhase_v2.5 Annual vehicle kilometrage, scenarios.	VrtS	vehicles: km/yr	None	Depending on the IAM	Regions Target Year Years step size km/yr per car	Use the same data for travelled distance per car per year	This dataset is used to relate the transport energy service with the fleet size of passengers cars. Usually IAMs assess the transport energy service, but not the fleet. If the later is done, the same km/yr/car must be used
6_MIP_VehicleOccupancyRate_V1.5 Occupancy rates for vehicles in different regions from 2015-2100. The rates are assumed to be uniform for all vehicle archetypes.	GrtS	1	None	Depending on the IAM	Regions Target Year Years step size Rate	Use the same occupancy rate	Some IAMs use occupancy rates for vehicles for different evaluations, rates must match between ODYM and IAM

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_10_Buildings_UsePhase_Historic_-V1.4 Share of m2 heated and cooled, historic age-cohorts	cBVrS	%	None	Depending on the IAM	Regions Target Year Years step size	Adjust during model calibration.	In the proposed integration for COFFEE, it is necessary to calibrate the data from the buildME simulation with historical data, and this process may alter these factors.
3_10_Buildings_UsePhase_Future_-Heating_V1.0 Share of m2 heated, future age-cohorts	GrtS	%	None	Depending on the IAM	Regions Target Year Years step size	Adjust during model calibration.	In the proposed integration for COFFEE, it is necessary to calibrate the data from the buildME simulation with historical data, and this process may alter these factors.
3_10_Buildings_UsePhase_Future_Cooling_V1.0 Share of m2 cooled, future age-cohorts	GrtS	%	None	Depending on the IAM	Regions Target Year Years step size	Adjust during model calibration.	In the proposed integration for COFFEE, it is necessary to calibrate the data from the buildME simulation with historical data, and this process may alter these factors.
3_10_NonResBuildings_UsePhase_V1.2 Share of m2 heated and cooled, future age-cohorts	cNVrS	%	None	Depending on the IAM	Regions Target Year Years step size	Adjust during model calibration.	In the proposed integration for COFFEE, it is necessary to calibrate the data from the buildME simulation with historical data, and this process may alter these factors.

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
4_TC_ResidentialEnergyEfficiency_-Default_V1.0 Useful to final energy conversion.	VRrnt	1	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same transfer coefficients.	If the IAM differentiates by regions, years, or other aspects, it should also be adapted accordingly.
4_TC_ResidentialEnergyEfficiency_-Scenario_Heating_V1.0 Useful to final energy conversion.	VRrntS	%	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same transfer coefficients.	If energy demand from buildings is disaggregately assessed on IAM, the transfer coefficient must match.
4_TC_ResidentialEnergyEfficiency_-Scenario_Cooling_V1.0 Useful to final energy conversion.	VRrntS	%	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same transfer coefficients.	If energy demand from buildings are disaggregately assessed on IAM, transfer coefficient must match.
4_TC_NonResEnergyEfficiency_Default_V1.0 Useful to final energy conversion.	VRrnt	1	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same transfer coefficients.	If the IAM differentiates by regions, years, or other aspects, it should also be adapted accordingly.
4_TC_NonResEnergyEfficiency_Scenario_Heating_V1.0 Useful to final energy conversion.	VRrntS	%	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same transfer coefficients.	If energy demand from buildings is disaggregately assessed on IAM, the transfer coefficient must match.

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
4_TC_NonResEnergyEfficiency_Scenario_Cooling_V1.0 Useful to final energy conversion.	VRrntS	%	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same transfer coefficients.	If energy demand from buildings are disaggregately assessed on IAM, transfer coefficient must match.
3_LT_RECC_ProductLifetime_passvehicles_V3.1 Lifetime distribution parameters	pr	yr	None	Depending on the IAM	Regions Target Year Years step size Lifetime	Use the same ditribution and distribution parameter	If appliances are assed in the CGE-IAM, the same data for lifetime (distribution and parameters) must be used
3_LT_RECC_ProductLifetime_resbuildings_V4.5 Lifetime distribution parameters	Brc	yr	None	Depending on the IAM	Regions Target Year Years step size Lifetime Types of nonres buildings	Use the same distribution and distribution parameter and the same list of residential buildings	If residential buildings are assed in the CGE-IAM, the same data for lifetime (distribution and parameters) must be used, as the same types of residential buildings. Some IAMs describe the construction sector in the energy demand side assessment, the types of buildings must match between ODYM and IAM

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_LT_RECC_ProductLifetime_NonRes-buildings_V1.3 Lifetime distribution parameters	Nrc	yr	None	Depending on the IAM	Regions Target Year Years step size Lifetime Types of nonres buildings	Use the same ditribution and distribution parameter and the same list of nonresidential buildings	If non residential buildings are assed in the CGE-IAM, the same data for lifetime (distribution and parameters) must be used, as the same types of non residential buildings. Some IAMs describe the construction sector in the energy demand side assessment, the type of buildings must match between ODYM and IAM
3_LT_RECC_ProductLifetime_appliances_V1.0 Lifetime distribution parameters	a	yr	None	Depending on the IAM	Regions Target Year Years step size Lifetime Types of applian.	Use the same ditribution and distribution parameter and the same list of appliances	If appliances are assed in the CGE-IAM, the same data for lifetime (distribution and parameters) must be used, as the same types of appliances used
3_LT_RECC_ProductLifetime_industry_V1.0 Lifetime distribution parameters	I	yr	None	Depending on the IAM	Regions Target Year Years step size Lifetime Types of techs	Use the same types of technologies, ditribution and distribution parameter for their lifetimes	This dataset is only for electricity generation industry

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
3_LT_RECC_ProductLifetime_nonres-buildings_g_V1.0 Lifetime distribution parameters	Noc	yr	None	Partial	Regions Target Year Years step size Lifetime Types of techs	Use the same types of technologies, ditribution and distribution parameter for their lifetimes	This dataset is only for electricity generation industry
3_MC_RECC_Buildings_V1.3 Material composition of stock	cmBr	kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings
3_MC_RECC_Vehicles_V1.1 Material composition of stock	cmpr	kg/unit	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in vehicles
3_MC_RECC_NonResBuildings_V2.0 Material composition of stock	cmNr	kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings
3_MC_RECC_Nonresbuildings_g_V1.0 Material composition of stock	mN	kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings
3_MC_RECC_appliances_V1.1 Material composition of stock	Im	kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings
3_MC_RECC_appliances_V1.1 Material composition of stock	oam	kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in appliances
3_MC_RECC_Buildings_Renovation_-Relative_V1.0 Additional renovation material, in % of existing material content of buildings	cmBr	1	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_MC_RECC_Buildings_Renovation_-Absolute_V1.0 Additional renovation material, in kg/m^2 added to existing material content of buildings	cmBr	kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings
3_MC_RECC_NonResBuildings_Renovation_Absolute_V1.0 Additional renovation material, in kg/m^2 added to existing material content of buildings	cmNr	kg/m2	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
3_MC_Elements_Materials_Existing-Stock_V2.3 Element composition of materials in existing stock	me	1 (kg/kg)	None	Partial	Regions Target Year Years step size		Elements listed are Al, C, Cr, Cu and Fe for different types of engineering materials as concrete, stainless steel, electric grade copper, etc
3_MC_Elements_Materials_Primary_-V2.3 Element composition of materials in primary materials	me	1 (kg/kg)	None	Partial	Regions Target Year Years step size		Elements listed are Al, C, Cr, Cu and Fe for different types of engineering materials as concrete, stainless steel, electric grade copper, etc
3_PR_RECC_CO2Price_SSP_32R_V2.1 (not used in current version of RECC)	RtrS	US$2005/ton	IAM	Yes	Regions Target Year Years step size CO2 price	Use the same CO2 price in IAM and ODYM	IAMs usually use CO2 price as na input to choose between different technologies, the value used must be the same (value is scenario dependent)

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
3_SHA_RECC_REStrategyScaleUp_-V3.4 This parameter quantifies the extent to which a given industry RE strategy will be implemented (%). It applies to all industry RE strategy parameter and is dependent on time t, socioeconomic scenario S, and climate policy scenario R.	RotS	1	None	Partial	Regions Target Year		This dataset is only used when RE scenarios are run
3_SHA_BuildingRenovationScaleUp_-V1.0 This parameter quantifies the extent to which a given renovation potential (MRP, in % of stock), will have been used in model year t (in %).	RotS	1	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
3_SHA_NonResBuildingRenovation-ScaleUp_V1.0 This parameter quantifies the extent to which a given renovation potential (MRP, in % of stock), will have been used in model year t (in %).	RotS	1	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
4_E1_ProcessEnergyIntensity_V3.2 Direct energy demand of material production	Pnto	MJ/kg	None	Depending on the IAM	Target Year Year step size	Use the same coefficient	Some IAMs have a material sector in which material demand is converted into energy demand, sometimes with descriptions of production routes. This factor should be the same and can be dynamic, depending on the set of routes chosen in a given period.

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
4_El_ManufacturingEnergyIntensity_V2.2 Energy intensity of manufacturing.	Fnco	MJ/kg	None	Depending on the IAM	Target Year Year step size	Use the same coefficient	Usually, IAMs do not assess the energy demand of manufacturing activities. If they do, the same factor should be used.
4_El_HydrogenEnergyDemand Energy demand (electricity for electrolysis) per hydrogen	Ynt	MJ/MJ	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	
3_El_SpecificEnergy_EnergyCarriers Energy content of energy carriers	n	kg/MJ	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	
4_PE_Carbon_for_Electricity_Generation Biogenic carbon emissions for different electricity generation technologies	In	ton/GJ	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	Compatibility can be achieved, but this is a result provided by the IAM, meaning the ODYM would not need to compute it.
4_PE_ProcessExtensions_Materials Process emissions per primary material produced.	Pxot	impact-eq/kg	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	IAMs can provide these emissions in an aggregated manner, while ODYM-RECC can offer a detailed breakdown by phase, product, etc.

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
4_PE_ProcessExtensions_Industry Process emissions per electricity generated (Industry: electricity generation technology)	Ixot	impact-eq/kWh	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	IAMs can provide these emissions in an aggregated manner, while ODYM-RECC can offer a detailed breakdown by phase, product, etc.
4_PE_ProcessExtensions_EnergyCarriers Process emissions per energy carrier supplied (other than electricity).	Nxot	impact-eq/kg	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	Compatibility can be achieved, but this is a result provided by the IAM, meaning the ODYM would not need to compute it.
4_SHA_ElectricityMix_World Average World electricity mix	oRlt	%	IAM	Yes	Regions Target Year Years step size	Use the same coefficient	
4_SHA_ElectricityMix_World_Alu Average World electricity mix, for aluminium industry only	oRlt	%	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	Only if the IAM contains and/or utilizes this data.
4_SHA_ElectricityMix Average regional electricity mix	rRlt	%	IAM	Yes	Regions Target Year Years step size Coefficient	Use the same coefficient	
4_SHA_MaterialsTechnologyShare Mix of different material production technologies in total material production.	otmRP	%	IAM	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same coefficient	Only if the IAM contains and/or utilizes this data.

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
4_PY_EOL_RecoveryRate_v2.5 End-of-life recovery rate of scrap from end-of-life products.	gomwW	%	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	An IAM rarely assesses metals EoL processes and recovery.
4_PY_Manufacturing_V2.4 Process yield in manufacturing, material into product.	mwgFto	1	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	An IAM rarely assesses material losses during processes.
4_PY_MaterialProductionRemelting_-v2.4 Process yield scrap into secondary material.	wmeWto	1	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	An IAM rarely assesses remelting process and it yields.
4_EI_WasteMgtEnergyIntensity_V1.1 Energy demand per mass of EoL product to be dismantled, shredded, and sorted.	wnco	MJ/kg	None	Depending on the IAM	Target Year Year step size	Use the same coefficient	Usually, IAMs do not assess the energy demand of EoL activities. If they do, the same factor should be used.
4_EI_RemeltingEnergyIntensity_V2.1 Energy demand per mass of secondary material produced from scrap.	mnco	MJ/kg	None	Depending on the IAM	Target Year Year step size	Use the same coefficient	Some IAMs have a material sector in which material demand is converted into energy demand, sometimes with descriptions of production routes. This factor should be the same and can be dynamic, depending on the set of routes chosen in a given period.
6_PR_EOL_RR_Improvement_v2.3 Percentage points of increase in EoL recovery rate.	gomwW	percentage points	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	An IAM rarely assesses EoL recovery rates.

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
6_PR_LifeTimeExtension_passvehicles_V2.1 Factor >= 1 that scales the current to the extended lifetime.	poS	1	None	Partial	Regions Target Year Years step size	Use the same LT dataset	This dataset is only used when RE scenarios are run. If this is the case, LTs used in ODYM must match those used in IAM
6_PR_LifeTimeExtension_resbuildings_v2.3 Factor >= 1 that scales the current to the extended lifetime.	BrS	1	None	Partial	Regions Target Year Years step size	Use the same LT dataset	This dataset is only used when RE scenarios are run. If this is the case, LTs used in ODYM must match those used in IAM
6_PR_LifeTimeExtension_nonresbuildings_V1.1 Factor >= 1 that scales the current to the extended lifetime.	Nr	1	None	Partial	Regions Target Year Years step size	Use the same LT dataset	This dataset is only used when RE scenarios are run. If this is the case, LTs used in ODYM must match those used in IAM
6_PR_LifeTimeExtension_nonresbuildings_g_V1.0 Factor >= 1 that scales the current to the extended lifetime.	No	1	None	Partial	Regions Target Year Years step size	Use the same LT dataset	This dataset is only used when RE scenarios are run. If this is the case, LTs used in ODYM must match those used in IAM
6_PR_LifeTimeExtension_industry_V1.0 Factor >= 1 that scales the current to the extended lifetime.	lIs	1	None	Partial	Regions Target Year Years step size	Use the same LT dataset	This dataset is only used when RE scenarios are run. If this is the case, LTs used in ODYM must match those used in IAM
6_PR_LifeTimeExtension_appliances_V1.0 Factor >= 1 that scales the current to the extended lifetime.	aoS	1	None	Partial	Regions Target Year Years step size	Use the same LT dataset	This dataset is only used when RE scenarios are run. If this is the case, LTs used in ODYM must match those used in IAM

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
6_PR_FabricationYieldImprovement_V2.1 Factor that indicates the maximum change from current to future fabrication yield.	mgoS	1	None	Depending on the IAM	Regions Target Year Years step size Yields	Use the same dataset for yields	An IAM rarely assesses yields on metals fabrication process, but some of then evaluate some material fabrication processes, if it is the case, data must match.
6_PR_FabricationScrapDiversion_V1.2 Factor that indicates the maximum share of all yield loss into re-use applications that don't require remelting.	mwoS	1	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	An IAM rarely assesses steal scrap management
6_PR_ReUse_Bld_V3.5 Share of recovered building material that is re-used as a component instead of being recycled by destruction.	mBo	1	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	This dataset is only used when RE scenarios are run.
6_PR_ReUse_Veh_V1.3 Reuse rates for different materials (e.g., % of cast Al from reuse of vehicle components) in 6 vehicle archetypes, from 2015 to 2100, for each region.	mprtS	1	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	This dataset is only used when RE scenarios are run.
6_PR_ReUse_nonresBld_V1.4 Share of recovered building material that is re-used as a component instead of being recycled by destruction.	mNo	1	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	This dataset is only used when RE scenarios are run.
6_PR_DirectEmissions_V1.2 Direct GHG from burning different energy carriers.	Xn	kg of CO2-eq/MJ	None	Yes	Regions Target Year Years step size Value	Use the same emissions factors and same primary energy supply types	IAMs assess GHG emissions from different energy supplies, this data must match.

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
6_PR_CarSharingShare_V1.3 Share of total passenger-km delivered by carsharing.	GotS	1	None	Depending on the IAM	Regions Target Year Years step size Share	Use the same share of carsharing	In any efficient scenario involving car sharing, the sharing ratio must remain consistent.
6_PR_RideSharingShare_V2.1 Percentage of transport service demand fulfilled by ride sharing from 2015 to 2100, assumed to be identical for all regions and all archetypes.	GrtS	1	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	This dataset is only used when RE scenarios are run.
3_SHA_TypeSplit_Vehicles_V3.0 Describes the split of vehicle types under different scenarios.	GrRpt	%	None	Yes	Regions Target Year Years step size Share	Use the same dataset in both ODYM and IAM	If CGE-IAM assess passenger vehicles and/or share of them to correspond to a transportation service, types of passenger vehicles and its shares must match. As mentioned above, ODYM database uses 6 different technologies for passenger vehicles (ICEG, ICED, BEV, HEV, PHEV, FCV)
3_SHA_TypeSplit_Buildings_V2.0 Describes the split of residential buildings by type and energy efficiency standard.	BrtSR	%	None	Yes	Regions Target Year Years step size Share	Use the same dataset in both ODYM and IAM	If CGE-IAM assess residential buildings, types of residential buildings and its shares must match

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_SHA_TypeSplit_NonResBuildings_-V3.0 Describes the split of nonresidential buildings by type and energy efficiency standard.	NrtS	%	None	Yes	Regions Target Year Years step size Share	Use the same dataset in both ODYM and IAM	If CGE-IAM assess non residential buildings, types of non residential buildings and its shares must match
3_SHA_EnergyCarrierSplit_Vehicles_-V1.1 Splits total driving energy demand into different energy carriers for vehicles.	cpoVnS	%	IAM	Depending on the IAM	Regions Target Year Years step size Types of Energy Carriers and Share	Use the same type of vehicles, the same share of energy carrier in vehicles consumption	Some IAMs model the energy demand sid Types of veh
3_SHA_EnergyCarrierSplit_Buildings_-V3.0 Describes the distribution of energy carriers used in residential buildings under different scenarios.	VRrnt	%	IAM	Depending on the IAM	Regions Target Year Years step size Types of Energy Carriers and Share	Use the same type of buildings, the same share of energy carrier in buildings consumption	Some IAMs model the energy demand sid Types of buil
3_SHA_EnergyCarrierSplit_NonRes-Buildings_V2.0 Describes the distribution of energy carriers in nonresidential buildings.	VRrnt	%	IAM	Depending on the IAM	Regions Target Year Years step size Types of Energy Carriers and Share	Use the same type of buildings, the same share of energy carrier in buildings consumption	Some IAMs model the energy demand sid Types of buil
3_MC_VehicleArchetypes_V2.0 Material composition of vehicle archetypes across different configurations.	Am	kg/unit, kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in vehicles

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
3_EL_VehicleArchetypes_V4.0 Fuel economy of vehicle archetypes derived from FASTSim.	An	MJ/km, MJ/m2/yr	None	Yes	Regions Target Year Years step size Energy Intensity	Use the same calculation methods and parameters for scenarios, regions, type of passenger vehicles and MJ/km ratios	The dataset includes 48 types of passenger vehicles, including 6 types of fueling (ICE-gasoline, ICE-diesel, HEV, PHEV, BEV, FCV), different sizes and design (SUV, microcar, light-truck, etc) combination. Compatibility between cars archetypes must be done.
3_MC_BuildingArchetypes_V2.0 Material composition of building archetypes, calculated based on sources like Taylor et al. 2015.	Arm	kg/unit, kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings
3_EL_BuildingArchetypes_V2.0 Energy intensity for various building types including residential space heating, cooling, and hot water.	ArVn	MJ/km, MJ/m2/yr	None	Yes	Regions Target Year Years step size Energy Use	If IAM assess energy demand by buildings, the same parameters should be used in ODYM and IAM	Some IAMs assess the energy demand for buildings, if this is the case, for compatibility purposes, ODYM and IAM must use the same parameters and calculation methods. ODYM uses a MJ per m2 of constructed area for different types of residential buildings, regions and energy vectors, this also should be used instead of IAM parametes

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_MC_NonResBuildingArchetypes_-V2.0 Material composition for non-residential buildings.	Arm	kg/unit, kg/m2	None	Partial	Regions Target Year Years step size		Presupposing that the IAM does not assess materials in buildings
3_EL_NonResBuildingArchetypes_V2.0 Energy intensity for non-residential buildings covering major energy services.	ArVn	MJ/km, MJ/m2/yr	None	Yes	Regions Target Year Years step size Energy Use	If IAM assess energy demand by buildings, the same parameters should be used in ODYM and IAM	Some IAMs assess the energy demand for buildings, if this is the case, for compatibility purposes, ODYM and IAM must use the same parameters and calculation methods. ODYM uses a MJ per m2 of constructed area for different types of buildings, regions and energy vectors, this also should be used instead of IAM parametes
3_SHA_DownSizing_Vehicles_V2.4 Market share of each vehicle size segment, assumed to change annually from 2015 to 2100.	srtS	%	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
8_FLAG_VehicleDownsizingDirection_-V1.0 Flag set for scenario case to lead lower GHG emissions.	rS	Bool	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	This dataset is only used when RE scenarios are run.
3_SHA_LightWeighting_Vehicles_V1.4 Market share of light-weighted vehicles per powertrain from 2015 to 2100.	prtS	%	None	Partial	Regions Target Year		This dataset is only used when RE scenarios are run

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_SHA_DownSizing_Buildings_V1.4 Share of new constructions considered in the lightweighting Material Efficiency Strategy.	urtS	%	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
3_SHA_LightWeighting_Buildings_V2.3 Share of new residential buildings built predominantly from timber.	GrtS	%	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
3_SHA_DownSizing_NonResBuildings_V1.1 Share of new nonresidential constructions considered in the lightweighting Material Efficiency Strategy.	urtS	%	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
3_SHA_LightWeighting_NonResBuildings_V1.1 Share of new nonresidential buildings built predominantly from timber.	GrtS	%	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
6_PR_Calibration_V2.5 Calibration values to scale energy intensity and vehicle operation.	Cr	ratios	None	Partial	Regions Target Year	Match regions and target year between ODYM and IAM	This is a dataset to calibrate and initialize MFA

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
6_MIP_CarSharing_Stock_V1.0 Ratio of per capita passenger vehicle stock with vs. without carsharing.	Sr	1	None	Depending on the IAM	Regions Target Year Years step size Share	Use the same share of carsharing	The coefficient correlates car sharing and stocks in comparison to a non-car sharing situation. While the IAM doesn't directly relate to stocks, in any efficient scenario involving car sharing, the sharing ratio must remain consistent.
6_MIP_RideSharing_Occupancy_V1.1 Occupancy rates for ride-sharing vehicles, uniform across all regions.	Sr	1	None	Partial	Regions Target Year		This dataset is only used in some RE scenarios strategies. In particular, factors are set 1 by defaut
6_MIP_GWP_Bio_V1.1 Characterisation factors for dynamic GWP of biogenic carbon.	c	1	None	Depending on the IAM	Regions Target Year Years step size Value	Use the same value for the potential of biomass with storage and incineration	0
3_SHA_MaxRenovationPotential_ResBuildings_V1.1 Potential estimates are in line with Burger et al. 2018.	rcB	1	None	Partial	Regions Target Year		This dataset is only used when RE scenarios are run
3_SHA_MaxRenovationPotential_NonResBuildings_V1.0 Potential estimates for non-residential buildings.	rcN	1	None	Partial	Regions Target Year		This dataset is only used when RE scenarios are run

Reference and Rationale	Aspect structure	Unit	New Input	Needs Compatibility	Which Aspects?	Compatibility Action Description	Comments
3_SHA_EnergySavingsPot_Renovation_ResBuildings_V1.1 Energy savings potential estimates for residential buildings.	rSB	1	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
3_SHA_EnergySavingsPot_Renovation_NonResBuildings_V1.1 Energy savings potential for non-residential buildings.	rSN	1	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
6_MIP_CharacterisationFactors_V2.1 Characterisation factors for environmental extensions.	xX	misc. units	None	Yes	Regions Target Year Years step size Factors	Use the same GWP factors	The dataset correlates different GWP with different GHG. ODYM and IAM must use the same dataset
6_MIP_Cumulative_Pressure_Indicators Cumulative characterisation factors for environmental extensions.	xUt	misc. units	None	Depending on the IAM	Regions Target Year Years step size Factors	Use the same GWP factors	Only if the IAM assesses this type of impact, which is not common.
4_PE_ElectricityFromWoodCombustion_V1.0 Electricity generated from wood combustion.	wWn	GJ/ton	None	Depending on the IAM	Regions Target Year Years step size Coefficient	Use the same value for the generated energy in ODYM and in IAM	If the IAM has that kind of factor in its internat equations, the number must match

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_LT_ForestRotationPeriod_FuelWood_V1.0 Forest rotation period for fuel wood.	n	yr	None	Depending on the IAM	Regions Target Year Years step size Value	Use the same value for the rotation period in ODYM and in IAM	If if the IAM has a land use module and it takes a forest rotation period for fuel wood, the data must match. ODYM uses a single value of 30 years for all regions and during all the time assessed
3_LT_ForestRotationPeriod_Timber_V1.0 Forest rotation period for timber.	m	yr	None	Depending on the IAM	Regions Target Year Years step size Value	Use the same value for the rotation period in ODYM and in IAM	If if the IAM has a land use module and it takes a forest rotation period for timber wood, the data must match. ODYM uses a single value of 70 years for all regions and during all the time assessed
3_MC_CO2FromWoodCombustion_V1.0 Average CO2 from burning a certain mass of wood.	xm	kgCO2/ kg wood	None	Yes	Regions Target Year Years step size CO2 emission	Match CO2 emission for wood combustion between IAM and ODYM	0
3_El_HeatingValueWoodPerCarbon_V1.0 Energy recovered from wood, per mass of carbon in wood.	em	MJ/kg	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run

Reference and Rationale	**Aspect structure**	**Unit**	**New Input**	**Needs Compatibility**	**Which Aspects?**	**Compatibility Action Description**	**Comments**
3_MC_CementContentConcrete_V1.0 Average cement content of concrete.	mm	1	None	Depending on the IAM	Regions Target Year Years step size Share	Match cement content of concrete between IAM and ODYM	Some IAMs assess cement and concrete production. If it uses some factor of the amount of cement in concrete, this data must match between IAM and ODYM
3_SHA_CementContentReduction_-V1.0 Reduction potential for the cement content.	m	misc. units	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
3_LT_Wood_Cascade Lifetime of recycled wood products in the cascade.	ou	yr	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
4_PY_TimberRoundWood Share of structural timber that is cut out of industrial roundwood logs.	rts	1	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
4_PY_WoodCascading Share of EoL wood products that enters a cascading use.	wmWr	1	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run
6_PR_WoodCascading_Improvement Improvement of the share of EoL wood products that enters a cascading use.	wmWr	pp	None	Partial	Regions Target Year Years step size		This dataset is only used when RE scenarios are run

I Annex I - The Convolution Sum and Convolution Integral

The Convolution Sum

Suppose a generic system that, in response to the input $x[n]$, provides the output $y[n]$. Consider the particular input $x[n] = \delta[n]$, that is, the input is a unit impulse sequence. The corresponding response will be called $y[n] = h[n]$. Thus, $h[n]$ is the response of a system to the unit impulse. It must be clear that $h[n]$ is the response to the impulse centered at $n = 0$. Now taking a generic sequence $x[n]$, we can write:

$$x[n] = \sum_{k=-\infty}^{\infty} x[k]\delta[n-k] \tag{I.1}$$

that is, $x[n]$ can be written as a linear combination of unit impulses. This sequence $x[n]$ will be the input to the system, producing $y[n]$ as output. Suppose the system is linear, then, as $x[n]$ is a linear combination of impulses, we can write $y[n]$ as a linear combination of impulse responses, that is,

$$y[n] = \sum_{k=-\infty}^{\infty} x[k]h_k[n], \tag{I.2}$$

where $h_k[n]$ is the response of the linear system to the impulse $\delta[n-k]$. Note that $h_k[n]$ is not equal to $h[n]$ since the corresponding impulse is not centered at the origin of the n axis.

Suppose that the system, in addition to being linear, is also time-invariant. In this case, we have $h_k[n] = h[n-k]$. Thus, the system's output can be rewritten as

$$y[n] = \sum_{k=-\infty}^{\infty} x[k]h[n-k]. \tag{I.3}$$

This is one of the most important properties of time-invariant linear systems: the output, in response to any input, can be calculated using the input and the system's impulse response. Therefore, the response $h[n]$ of a time-invariant linear system completely characterizes the system. The calculation expressed in I.3 is called the convolution sum and is represented by

$$y[n] = x[n] * h[n]. \tag{I.4}$$

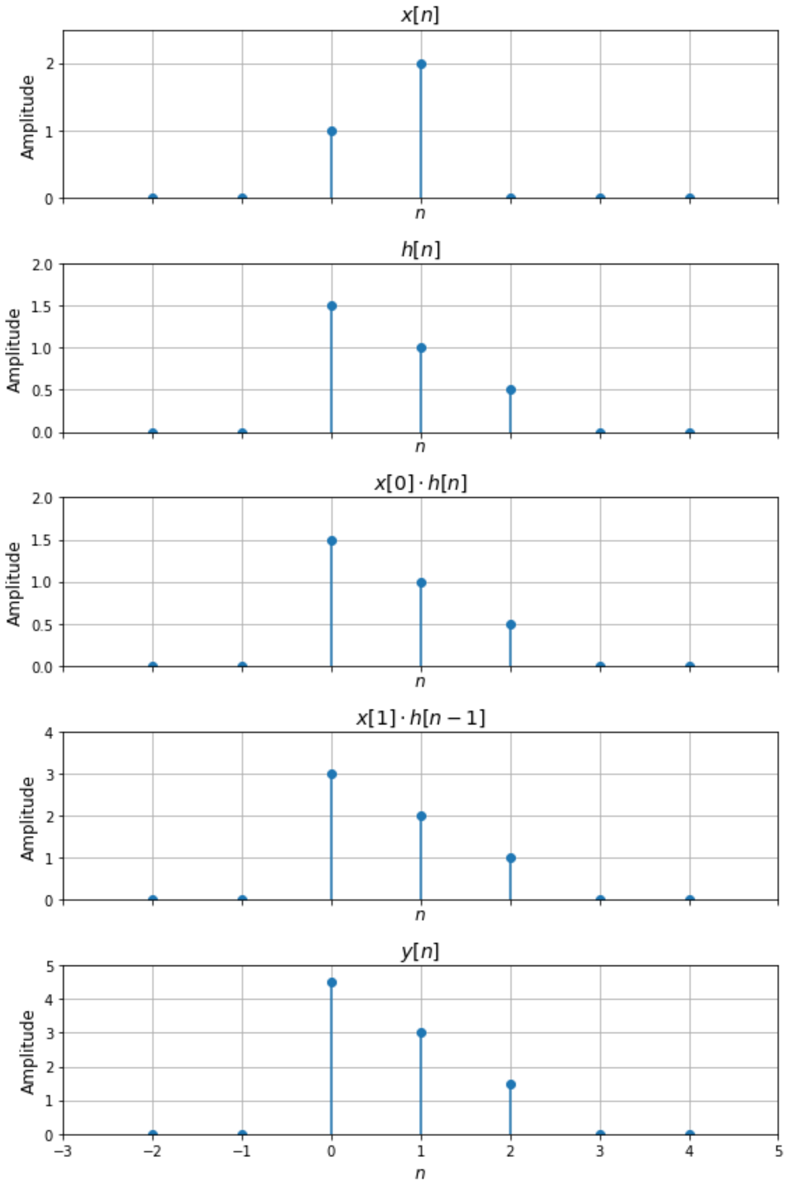

Figure I.1: Example of a convolution sum of a impulse series function as input

We will deduce a relationship between the impulse response, the input, and the output of a continuous LTI system, similar to that deduced for discrete systems. For this, we need the expression (2.30) from Chapter 2, repeated below, which explicitly states the sampling property of the unit impulse. [1]

[1]This annex was based on OPPENHEIM *et al.* (1996)

The Convolution Integral

To deduce the relationship between the convolution sum and integral, we start from the following equation, the derivation of which can be found in (OPPENHEIM *et al.*, 1996, p.93).

$$\int_{-\infty}^{\infty} x(\tau)\delta(t-\tau)\,d\tau = x(t). \tag{I.5}$$

Considering Figure I.2, the approximation $x_\Delta(t)$ of the function $x(t)$ can be written as:

$$x_\Delta(t) = \sum_{k=-\infty}^{\infty} x(k\Delta)\delta_\Delta(t-k\Delta)\Delta, \tag{I.6}$$

where $\delta_\Delta(t)$ is the function used in Chapter 2 to define the unit impulse. It can be shown that

$$\lim_{\Delta\to 0} x_\Delta(t) = x(t). \tag{I.7}$$

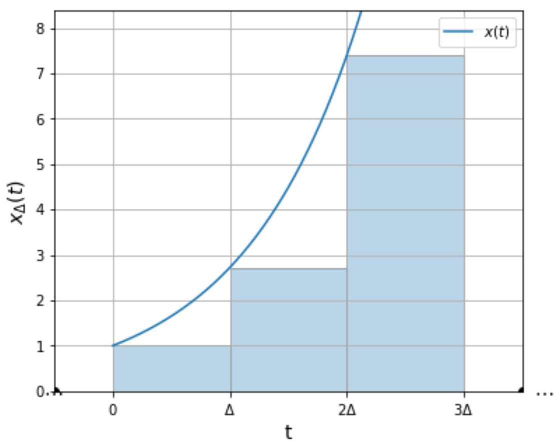

Figure I.2: Approximation of $x(t)$

Therefore,

$$x(t) = \lim_{\Delta\to 0} \sum_{k=-\infty}^{\infty} x(k\Delta)\delta_\Delta(t-k\Delta)\Delta. \tag{I.8}$$

However, in the limit $k\Delta \to \tau$, $\Delta \to d\tau$, $\delta_\Delta(t-k\Delta) \to \delta(t-\tau)$, and $\sum \to \int$. Therefore,

$$x(t) = \int_{-\infty}^{\infty} x(\tau)\delta(t-\tau)\,d\tau \tag{I.9}$$

Now, consider a LTI for which the input $\delta_\Delta(t)$ produces the output $h_\Delta(t)$, then, by the hypothesis of time invariance, we can state that the input $\delta_\Delta(t-k\Delta)$ will produce the output $h_\Delta(t-k\Delta)$. Suppose that $x_\Delta(t)$ from I.6 produces $y_\Delta(t)$ at the system output. Since $x_\Delta(t)$ is a linear combination of functions $\delta_\Delta(t-k\Delta)$, then the property of linearity allows us to write

$$y_\Delta(t) = \sum_{k=-\infty}^{\infty} x(k\Delta)h_\Delta(t-k\Delta)\Delta, \tag{I.10}$$

where $h_\Delta(t-k\Delta)$ is the response to $\delta_\Delta(t-k\Delta)$. But

$$\lim_{\Delta\to 0} x_\Delta(t) = x(t), \tag{I.11}$$

which implies

$$\lim_{\Delta\to 0} y_\Delta(t) = y(t), \tag{I.12}$$

since, by hypothesis, $x(t) \to y(t)$.

Therefore,

$$y(t) = \lim_{\Delta\to 0} \sum_{k=-\infty}^{\infty} x(k\Delta)h_\Delta(t-k\Delta)\Delta. \tag{I.13}$$

In the limit, we have

$$y(t) = \int_{-\infty}^{\infty} x(\tau)h(t-\tau)\,d\tau. \tag{I.14}$$

We conclude that the output of any continuous-time linear and time-invariant system can be calculated by knowing its impulse response. The integral operation involved in this response and the input is called the convolution integral.

This is the most important result for continuous LTI systems, just as it was for discrete systems.

Given the importance of the convolution integral, a special compact representation has been created for it. The convolution integral between the signal $x(t)$ and the signal $h(t)$, defined in expression 3.12, is represented by

$$y(t) = x(t) * h(t). \tag{I.15}$$

It is possible to demonstrate that

$$y(t) = \int_{-\infty}^{\infty} x(\tau)h(t-\tau)\,d\tau = \int_{-\infty}^{\infty} h(\tau)x(t-\tau)\,d\tau, \tag{I.16}$$

or, equivalently,

$$y(t) = x(t) * h(t) = h(t) * x(t). \tag{I.17}$$

II Annex II - Industrial Routes in COFFEE

The figures below present the industrial routes in COFFEE. The figure was produced by ZOTIN (2024).

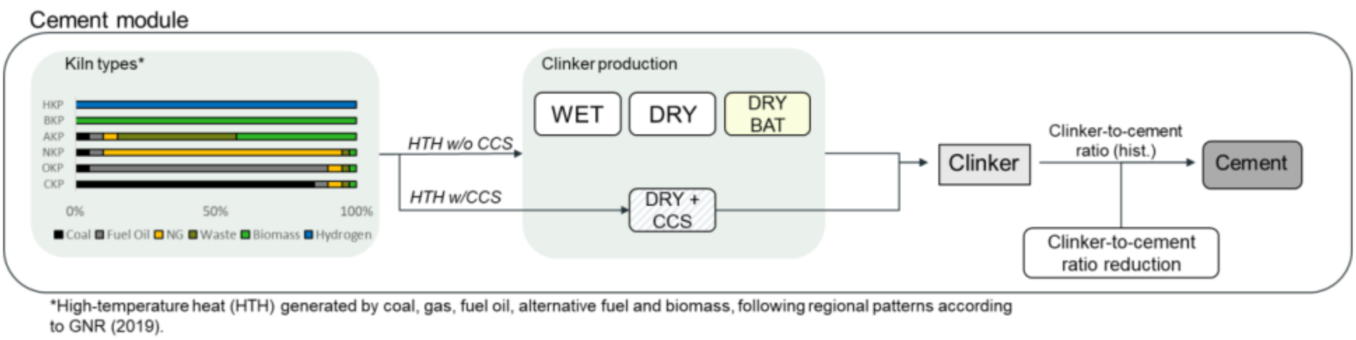

Figure II.1: Cement Routes in COFFEE. Source (ZOTIN, 2024)

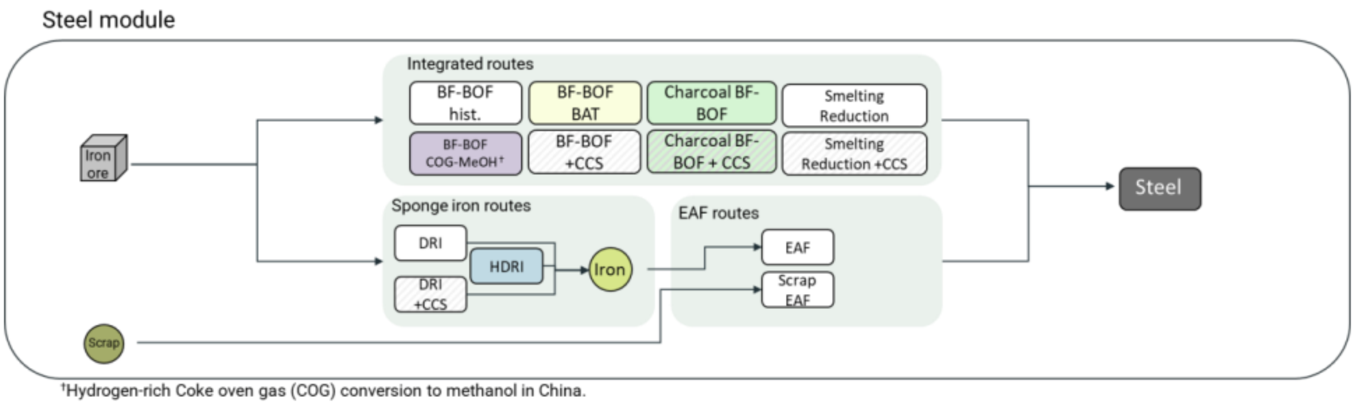

Figure II.2: Steel Routes in COFFEE. Source (ZOTIN, 2024)

Legend:

- BDH - Bioethanol Dehydration
- BGS - Biomass Gasification
- BF - Blast Furnace
- BOF - Blast Oxygen Furnace
- BTX - Benzene, Toluene, and Xylenes

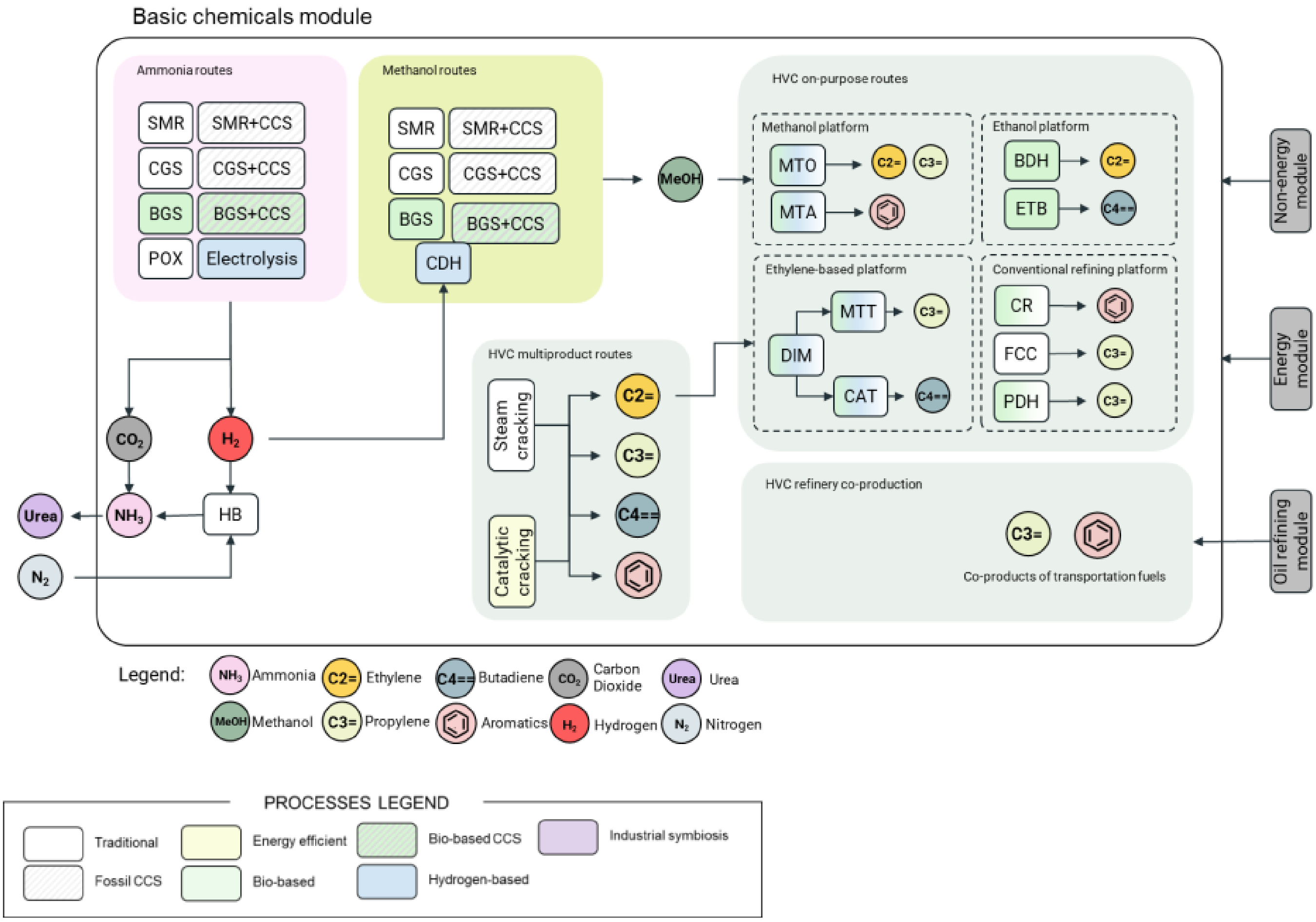

Figure II.3: Chemicals Routes in COFFEE. Source (ZOTIN, 2024)

- CAT - Catadiene®
- CDH - Carbon Dioxide Hydrogenation
- CDR - Carbon Dioxide Removal
- CGS - Coal Gasification
- CR - Catalytic Reforming
- DRI - Direct Reduced Iron
- EAF - Electric Arc Furnace
- ETB - Ethanol-to-Butadiene
- FCC - Fluidized Catalytic Cracking
- HB - Haber Bosch synthesis
- HDRI - Hydrogen Direct Reduced Iron
- HTH - High Temperature Heating
- MTA - Methanol-to-Aromatics
- MTO - Methanol-to-Olefins
- MTT - Metathesis
- PDH - Propane Dehydrogenation
- POX - Partial Oil Oxidation
- SMR - Steam Methane Reforming

III Annex III - Flows, Stocks and Outputs declared in ODYM-RECC

```
# Define system variables: Flows.
RECC_System.FlowDict['F_0_1'] = msc.Flow(Name='CO2 uptake',
  P_Start=0, P_End=1, Indices='t,r,e', Values=None, Uncert=None,
  Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_1_2'] = msc.Flow(Name='harvested wood',
  P_Start=1, P_End=2, Indices='t,r,e', Values=None, Uncert=None,
  Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_2_3'] = msc.Flow(Name='timber consumed by
   sawmills', P_Start=2, P_End=3, Indices='t,m,e', Values=None,
  Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_2_7'] = msc.Flow(Name='wood fuel use',
  P_Start=2, P_End=7, Indices='t,e', Values=None, Uncert=None,
  Color=None, ID=None, UUID=None) # flow is directly routed to use
   phase.
RECC_System.FlowDict['F_7_0'] = msc.Flow(Name='wood fuel use
  direct emissions', P_Start=7, P_End=0, Indices='t,e', Values=
  None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_0_3'] = msc.Flow(Name='ore input',
  P_Start=0, P_End=3, Indices='t,m,e', Values=None, Uncert=None,
  Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_3_4'] = msc.Flow(Name='primary material
  production', P_Start=3, P_End=4, Indices='t,m,e', Values=None,
  Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_3_10'] = msc.Flow(Name='primary material
  production waste', P_Start=3, P_End=10, Indices='t,r,w,e',
  Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_4_5'] = msc.Flow(Name='primary material
  consumption', P_Start=4, P_End=5, Indices='t,m,e', Values=None,
  Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_5_6'] = msc.Flow(Name='manufacturing
  output', P_Start=5, P_End=6, Indices='t,o,g,m,e', Values=None,
  Uncert=None, Color=None, ID=None, UUID=None)
```

```
RECC_System.FlowDict['F_6_7'] = msc.Flow(Name='final consumption', P_Start=6, P_End=7, Indices='t,r,g,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_6_7_Nl'] = msc.Flow(Name='final consumption Nl', P_Start=6, P_End=7, Indices='t,l,L,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_6_7_No'] = msc.Flow(Name='final consumption No', P_Start=6, P_End=7, Indices='t,o,O,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_7_8'] = msc.Flow(Name='EoL products', P_Start=7, P_End=8, Indices='t,c,r,g,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_7_8_Nl'] = msc.Flow(Name='EoL products Nl', P_Start=7, P_End=8, Indices='t,c,l,L,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_7_8_No'] = msc.Flow(Name='EoL products No', P_Start=7, P_End=8, Indices='t,c,o,O,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_0'] = msc.Flow(Name='obsolete stock formation', P_Start=8, P_End=0, Indices='t,c,r,g,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_0_Nl'] = msc.Flow(Name='obsolete stock formation Nl', P_Start=8, P_End=0, Indices='t,c,l,L,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_0_No'] = msc.Flow(Name='obsolete stock formation No', P_Start=8, P_End=0, Indices='t,c,o,O,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_9'] = msc.Flow(Name='waste mgt. input', P_Start=8, P_End=9, Indices='t,r,g,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_9_Nl'] = msc.Flow(Name='waste mgt. input Nl', P_Start=8, P_End=9, Indices='t,l,L,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_9_No'] = msc.Flow(Name='waste mgt. input No', P_Start=8, P_End=9, Indices='t,o,O,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_17'] = msc.Flow(Name='product re-use in', P_Start=8, P_End=17, Indices='t,c,r,g,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_17_Nl'] = msc.Flow(Name='product re-use in Nl', P_Start=8, P_End=17, Indices='t,c,l,L,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_8_17_No'] = msc.Flow(Name='product re-use in No', P_Start=8, P_End=17, Indices='t,c,o,O,m,e', Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_17_6'] = msc.Flow(Name='product re-use out', P_Start=17, P_End=6, Indices='t,c,r,g,m,e', Values=None,
```

```
    Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_17_6_Nl'] = msc.Flow(Name='product re-use
    out', P_Start=17, P_End=6, Indices='t,c,l,L,m,e', Values=None,
    Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_17_6_No'] = msc.Flow(Name='product re-use
    out', P_Start=17, P_End=6, Indices='t,c,o,O,m,e', Values=None,
    Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_9_10'] = msc.Flow(Name='old scrap',
    P_Start=9, P_End=10, Indices='t,r,w,e', Values=None, Uncert=None
    , Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_9_10_Nl'] = msc.Flow(Name='old scrap Nl',
    P_Start=9, P_End=10, Indices='t,l,w,e', Values=None, Uncert=
    None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_9_10_No'] = msc.Flow(Name='old scrap No',
    P_Start=9, P_End=10, Indices='t,o,w,e', Values=None, Uncert=
    None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_5_10'] = msc.Flow(Name='new scrap',
    P_Start=5, P_End=10, Indices='t,o,w,e', Values=None, Uncert=None
    , Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_10_9'] = msc.Flow(Name='scrap use',
    P_Start=10, P_End=9, Indices='t,o,w,e', Values=None, Uncert=None
    , Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_10_9w'] = msc.Flow(Name='wood waste use',
    P_Start=10, P_End=9, Indices='t,r,w,e', Values=None, Uncert=
    None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_9_12'] = msc.Flow(Name='secondary
    material production', P_Start=9, P_End=12, Indices='t,o,m,e',
    Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_10_12'] = msc.Flow(Name='
    fabscrapdiversion', P_Start=10, P_End=12, Indices='t,o,m,e',
    Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_12_5'] = msc.Flow(Name='secondary
    material consumption', P_Start=12, P_End=5, Indices='t,o,m,e',
    Values=None, Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_12_0'] = msc.Flow(Name='excess secondary
    material', P_Start=12, P_End=0, Indices='t,o,m,e', Values=None,
    Uncert=None, Color=None, ID=None, UUID=None)
RECC_System.FlowDict['F_9_0'] = msc.Flow(Name='waste mgt. and
    remelting losses', P_Start=9, P_End=0, Indices='t,e', Values=
    None, Uncert=None, Color=None, ID=None, UUID=None)
```

Listing III.1: List of Flows declared in ODYM-RECC

```
# Define system variables: Stocks.
RECC_System.StockDict['dS_0'] = msc.Stock(Name='System
    environment stock change', P_Res=0, Type=1, Indices='t,e',
    Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_1t'] = msc.Stock(Name='Forestry stock
```

```
change, timber', P_Res=1, Type=1, Indices='t,r,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_1t'] = msc.Stock(Name='Forestry carbon stock, timber', P_Res=1, Type=0, Indices='t,c,r,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_1f'] = msc.Stock(Name='Forestry stock change, fuel wood', P_Res=1, Type=1, Indices='t,r,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_1f'] = msc.Stock(Name='Forestry carbon stock, fuel wood', P_Res=1, Type=0, Indices='t,c,r,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_7'] = msc.Stock(Name='In-use stock', P_Res=7, Type=0, Indices='t,c,r,g,m,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_7_Nl'] = msc.Stock(Name='In-use stock', P_Res=7, Type=0, Indices='t,c,l,L,m,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_7_No'] = msc.Stock(Name='In-use stock', P_Res=7, Type=0, Indices='t,c,o,O,m,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_7'] = msc.Stock(Name='In-use stock change', P_Res=7, Type=1, Indices='t,c,r,g,m,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_7_Nl'] = msc.Stock(Name='In-use stock change', P_Res=7, Type=1, Indices='t,c,l,L,m,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_7_No'] = msc.Stock(Name='In-use stock change', P_Res=7, Type=1, Indices='t,c,o,O,m,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_9'] = msc.Stock(Name='Wood cascading buffer', P_Res=9, Type=0, Indices='t,c,r,w,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_9'] = msc.Stock(Name='Wood cascading buffer change', P_Res=9, Type=1, Indices='t,c,r,w,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_10'] = msc.Stock(Name='Fabrication scrap buffer', P_Res=10, Type=0, Indices='t,c,o,w,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_10'] = msc.Stock(Name='Fabrication scrap buffer change', P_Res=10, Type=1, Indices='t,o,w,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['S_10w'] = msc.Stock(Name='Wood waste buffer', P_Res=10, Type=0, Indices='t,c,r,w,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_10w'] = msc.Stock(Name='Wood waste buffer change', P_Res=10, Type=1, Indices='t,r,w,e', Values=None, Uncert=None, ID=None, UUID=None)
```

```
RECC_System.StockDict['S_12'] = msc.Stock(Name='secondary material buffer', P_Res=12, Type=0, Indices='t,o,m,e', Values=None, Uncert=None, ID=None, UUID=None)
RECC_System.StockDict['dS_12'] = msc.Stock(Name='Secondary material buffer change', P_Res=12, Type=1, Indices='t,o,m,e', Values=None, Uncert=None, ID=None, UUID=None)

```

Listing III.2: List of Stocks declared in ODYM-RECC

```
 #Define arrays for result export:
Impacts_System_13579di                    = np.zeros((Nx,Nt,NS,NR))
Impacts_System_3579di                     = np.zeros((Nx,Nt,NS,NR))
Impacts_UsePhase_7d                       = np.zeros((Nx,Nt,NS,NR))
Impacts_OtherThanUsePhaseDirect           = np.zeros((Nx,Nt,NS,NR))
Impacts_Materials_3di_9di                 = np.zeros((Nx,Nt,NS,NR)) # all processes and their energy supply chains except for manufacturing and use phase
Impacts_Vehicles_Direct                   = np.zeros((Nx,Nt,Nr,NS,NR))  # use phase only
Impacts_ReBuildgs_Direct                  = np.zeros((Nx,Nt,Nr,NS,NR))  # use phase only
Impacts_NRBuildgs_Direct                  = np.zeros((Nx,Nt,Nr,NS,NR))  # use phase only
Impacts_NRBuildgs_Direct_g                = np.zeros((Nx,Nt,NS,NR)) # use phase only
Impacts_Vehicles_indir                    = np.zeros((Nx,Nt,NS,NR)) # energy supply only
Impacts_AllBuildings_indir                = np.zeros((Nx,Nt,NS,NR)) # energy supply only
Impacts_Manufact_5di_all                  = np.zeros((Nx,Nt,NS,NR))
Impacts_WasteMgt_9di_all                  = np.zeros((Nx,Nt,NS,NR))
Impacts_PrimaryMaterial_3di               = np.zeros((Nx,Nt,NS,NR))
Impacts_PrimaryMaterial_3di_m             = np.zeros((Nx,Nt,Nm,NS,NR))
Impacts_SecondaryMetal_di_m               = np.zeros((Nx,Nt,Nm,NS,NR))
Impacts_UsePhase_7i_Scope2_El             = np.zeros((Nx,Nt,NS,NR))
Impacts_UsePhase_7i_OtherIndir            = np.zeros((Nx,Nt,NS,NR))
Impacts_MaterialCycle_5di_9di             = np.zeros((Nx,Nt,NS,NR))
Impacts_RecyclingCredit                   = np.zeros((Nx,Nt,NS,NR))
Impacts_ForestCO2Uptake                   = np.zeros((Nx,Nt,NS,NR))
Impacts_ForestCO2Uptake_r                 = np.zeros((Nx,Nt,Nr,NS,NR))
Impacts_EnergyRecoveryWasteWood           = np.zeros((Nx,Nt,NS,NR))
Impacts_ByEnergyCarrier_UsePhase_d        = np.zeros((Nx,Nt,Nr,Nn,NS,NR))
Impacts_ByEnergyCarrier_UsePhase_i        = np.zeros((Nx,Nt,Nr,Nn,NS,NR))
Impacts_Energy_Supply_All                 = np.zeros((Nx,Nt,NS,NR)) # impacts of all energy carriers for all processes.
```

```python

dynGWP_System_3579di                    = np.zeros((NS,NR)) # dynGWP100 of entire system
dynGWP_WoodCycle                        = np.zeros((NS,NR)) # dynGWP100 of wood use: forest uptake + wood-related emissions from waste mgt. Pos sign for flow from system to environment.

Material_Inflow                     = np.zeros((Nt,Ng,Nm,NS,NR))
Scrap_Outflow                       = np.zeros((Nt,Nw,NS,NR))
PrimaryProduction                   = np.zeros((Nt,Nm,NS,NR))
SecondaryProduct                    = np.zeros((Nt,Nm,NS,NR))
SecondaryExport                     = np.zeros((Nt,Nm,NS,NR))
SecondaryProduct_EoL_Pot            = np.zeros((Nt,Nm,NS,NR)) # Secondary material from EoL material flows only, part of F_9_12, for reporting only
RenovationMaterialInflow_7          = np.zeros((Nt,Nm,NS,NR))
Element_Material_Composition        = np.zeros((Nt,Nm,Ne,NS,NR))
Element_Material_Composition_raw = np.zeros((Nt,Nm,Ne,NS,NR))
Element_Material_Composition_con = np.zeros((Nt,Nm,Ne,NS,NR))
Manufacturing_Output                = np.zeros((Nt,Ng,Nm,NS,NR))
StockMatch_2015                     = np.zeros((NG,Nr))
NegInflowFlags                      = np.zeros((NS,NR))
#NegInflowFlags_After2020            = np.zeros((NS,NR))
FabricationScrap                    = np.zeros((Nt,Nw,NS,NR))
EnergyCons_UP_Vh                    = np.zeros((Nt,NS,NR))
EnergyCons_UP_Bd                    = np.zeros((Nt,NS,NR))
EnergyCons_Mn                       = np.zeros((Nt,NS,NR))
EnergyCons_Wm                       = np.zeros((Nt,NS,NR))
EnergyCons_PP                       = np.zeros((Nt,NS,NR))
EnergyCons_PP_m                     = np.zeros((Nt,Nm,NS,NR))
EnergyCons_UP_serv_pav              = np.zeros((Nt,Nr,NV,NS,NR))
EnergyCons_UP_serv_reb              = np.zeros((Nt,Nr,NV,NS,NR))
EnergyCons_UP_serv_nrb              = np.zeros((Nt,Nr,NV,NS,NR))
EnergyCons_UP_total                 = np.zeros((Nt,Nn,NS,NR))
EnergyCons_UP_reb                   = np.zeros((Nt,Nn,NS,NR))
EnergyCons_UP_nrb                   = np.zeros((Nt,Nn,NS,NR))
EnergyCons_total                    = np.zeros((Nt,Nn,NS,NR))
StockCurves_Totl                    = np.zeros((Nt,NG,NS,NR))
StockCurves_Prod                    = np.zeros((Nt,Ng,NS,NR))
StockCurves_Mat                     = np.zeros((Nt,Nm,NS,NR))
StockCurves_Mat_reb                 = np.zeros((Nt,Nm,NS,NR))
StockCurves_Mat_nrb                 = np.zeros((Nt,Nm,NS,NR))
Inflow_Prod                         = np.zeros((Nt,Ng,NS,NR))
Inflow_Prod_r                       = np.zeros((Nt,Nr,Ng,NS,NR))
Outflow_Prod                        = np.zeros((Nt,Ng,NS,NR))
Outflow_Prod_r                      = np.zeros((Nt,Nr,Ng,NS,NR))
EoL_Products_for_WasteMgt           = np.zeros((Nt,Ng,NS,NR))
```

```
Outflow_Materials_Usephase_all   = np.zeros((Nt,Nm,NS,NR))
Outflow_Products_Usephase_all    = np.zeros((Nt,Ng,NS,NR))
WasteMgtLosses_To_Landfill       = np.zeros((Nt,Ne,NS,NR))
Population                       = np.zeros((Nt,Nr,NS,NR))
pCStocksCurves                   = np.zeros((Nt,NG,Nr,NS,NR))
Passenger_km                     = np.zeros((Nt,NS,NR))
Vehicle_km                       = np.zeros((Nt,NS,NR))
Service_IO_ResBuildings          = np.zeros((Nt,NV,NS,NR))
Service_IO_NonResBuildings       = np.zeros((Nt,NV,NS,NR))
ReUse_Materials                  = np.zeros((Nt,Nm,NS,NR))
Carbon_IndustrialRoundwood_bld   = np.zeros((Nt,Nr,NS,NR)) # Industrial roundwood, hard and softwood, for processing into structural wood elements for residential and non-residential buildings. Unit: Mt/yr of C.
Carbon_Fuelwood_bld              = np.zeros((Nt,NS,NR)) # Fuelwood, hard and softwood, for use in building heating and hot water only (no cooking fuel).
Carbon_Fuelwood_el               = np.zeros((Nt,NS,NR)) # Fuelwood, hard and softwood, for use in electricity generation.
Carbon_Fuelwood_release          = np.zeros((Nt,NS,NR)) # Total wood C outflow from fuelwood, in form of CO2.
Carbon_Wood_Inflow               = np.zeros((Nt,Nr,NS,NR))
Carbon_Wood_Outflow              = np.zeros((Nt,Nr,NS,NR))
Carbon_Wood_Stock                = np.zeros((Nt,Nr,NS,NR))
Cement_Inflow                    = np.zeros((Nt,Nr,NS,NR))
Vehicle_FuelEff                  = np.zeros((Nt,Np,Nr,NS,NR))
ResBuildng_EnergyCons            = np.zeros((Nt,NB,Nr,NS,NR))
GWP_bio_Credit                   = np.zeros((Nt,NS,NR))
EnergySubst_WtE_EL               = np.zeros((Nt,NS,NR))
EnergySubst_WtE_NG               = np.zeros((Nt,NS,NR))
FuelWoodSubst_WoodWaste          = np.zeros((Nt,NS,NR))
BiogenicCO2WasteCombustion       = np.zeros((Nt,NS,NR))
SysVar_RoundwoodConstruc_c_1_2_r = np.zeros((Nt,Nr,NS,NR))
SysVar_WoodWasteIncineration     = np.zeros((Nt,Nr,Nw,Ne,NS,NR))
SysVar_EoLCascEntry              = np.zeros((Nt,Nr,NS,NR))
SysVar_CascadeRelease            = np.zeros((Nt,Nr,Nw,Ne,NS,NR))
SysVar_WoodWaste_Gas_El          = np.zeros((Nt,Nr,NS,NR))
WoodCascadingInflow              = np.zeros((Nt,Nr,NS,NR))
WoodCascadingStock               = np.zeros((Nt,Nr,NS,NR))
Stock_2020_pav                   = np.zeros((Nt,Nr,NS,NR))
Stock_2020_reb                   = np.zeros((Nt,Nr,NS,NR))
Stock_2020_nrb                   = np.zeros((Nt,Nr,NS,NR))
NegInflowFlags                   = np.zeros((NG,NS,NR))
time_dsm                         = np.arange(0,Nc,1) # time array of [0:Nc) needed for some sectors
```

Listing III.3: List of Secondary outputs declared in ODYM-RECC