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BUILDING A LOW-CARBON, CLIMATE RESILIENT FUTURE:

SECURE, CLEAN AND EFFICIENT ENERGY

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SENTINEL

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1 Introduction: The need for environmental assessment in energy modelling

The EU Energy Union Strategy (COM/2015/080) calls for a decarbonisation of the energy system that allows Member States to meet the commitments of the Paris Agreement. Indeed, decarbonisation of the energy system is one of the five pillars of the strategy. More recent documents, such as (European Commission 2020) and (European Council 2020) have presented specific emission reduction targets for the EU for 2030 and 2050. A decarbonised, renewable energy system is used as a synonym of a clean and sustainable one but renewable, "decarbonised" energy systems have many other impacts over the environment (Akella et al. 2009). In the two documents that form the communication the words "water", "biodiversity" or "raw materials" do not appear. Ignoring the trade-offs between energy systems and other resources can result in misleading information and misguided policy making (Brouwer et al. 2018). Consequently, it has been suggested that the definition of sustainable energy transition pathways should consider the trade-offs between resources and other environmental impacts beyond air emissions (Von Stechow et al. 2016).

Administrations use energy system models (ESMs) for prospective energy scenario design. ESMs have not been very good at predicting the future of renewable energy nor at including sustainability dimensions (Nikas et al. 2021). In order to solve the first issue, it has been proposed to move away from one-size-fits-all models into modelling platforms that can soft link more specific models and that can be tailored to the specifics of the system under consideration (Nikas et al. 2021). However, the *issue of including sustainability in ESM remains unresolved* and many administrations are not in the position of valuing systemic environmental effects of energy policies due to this lack.

Some efforts have been made to evaluate the sustainability of energy systems mostly from the area of integrated assessment (IA) and Life Cycle Assessment (LCA). IA modelling suits are formed by a number of specific model interconnected in order to assess how changes in one would affect the other one. They have been criticised, among others, for being opaque (Pfenninger 2017) and lacking the full value chain perspective.

Life cycle assessment (LCA) has been used to assess the environmental impacts related to the value chain of renewable energy systems, mostly for emissions, raw materials and land use(Singh et al. 2014, Lausselet et al. 2017, Oreggioni et al. 2017, Dai et al. 2019, Li et al. 2019, Hollingsworth et al. 2020) Most of these analyses refer to a functional unit of 1 KWh, which is useful to compared different energy systems. However, they do not provide information on emergent, systemic impacts of the system once this is implemented. To do this, an upscaling of LCA results is necessary, which considers the complex configuration of socio-ecosystems (Creutzig et al. 2012).

The multi-scale integrated assessment of socio-ecosystem metabolism (MuSIASEM) (Giampietro et al. 2009) is a methodological framework for the assessment of water-food-energy trade-offs that considers the complex configuration of socio-ecosystems (Giampietro et al. 2014a). It has been extensively used to assess the bioeconomic viability of social systems, with a particular focus on energy systems (Giampietro et al. 2014b). MuSIASEM's environmental impact assessment is mostly related to water systems (Madrid-López et al. 2014) and still theoretical (Lomas and Giampietro 2017, Serrano-Tovar et al. 2019). Its further development into a more applied framework requires the integration with other tools that provide environmental assessment capabilities, like LCA.

In SENTINEL we integrated the value-chain and environmental assessment capabilities of LCA with the systemic approach of MuSIASEM to assess the environmental impacts and biophysical constraints of the renewable energy transition. The challenge of this integration is posed by the link between the structural, technology-based approach of LCA with the functional, sectorial-based approach of MuSIASEM. Some efforts have been developed within the MuSIASEM community to connect functions and structures in the assessment of sequential pathways (Di Felice et al. 2019, Parra et al. 2020) without an actual integration with LCA methods or data.

The LCA-MuSIASEM integration is challenged by an internal and an external factor. The internal factor is the intrinsic difficulties of integrating different modelling semantics (Kovacic 2017). The external factor is the need to include a variety of user needs in the modelling semiotic process (Sebeok and Danesi 2012, Ellenbeck and Lilliestam 2019, Silvast et al. 2020). To deal with this challenges, the integration of LCA and MuSIASEM into a framework has been developed considering the semantics of the SENTINEL energy models and the needs of the decision makers that will use the resulting information.

This framework is the basis of ENBIOS[1], a Python package developed as the environmental assessment module of the SENTINEL platform. Designed to enable the holistic evaluation of the environmental impacts and other metabolic factors associated with reaching the projected emissions targets for the EU by 2030 and 2050, ENBIOS is the only module that has been fully developed within SENTINEL. During the development of ENBIOS, the perspective of energy modellers and end users of the resulting information have been considered in an attempt to do the process as collaborative as possible. Co-creative approaches gained increasing relevance in modelling, to ensure models' fit-for-purpose, to increase model credibility and legitimacy, and to accelerate modelling impact in policy (van Daalen et al. 2002, Voinov and Bousquet 2010, Renn 2015, Van Ittersum and Sterk 2015, McDowall and Geels 2017).

The remaining of the document explains what user needs and modelling semantics have been included, the methodological integration of LCA and MuSIASEM and the formalization into the ENBIOS code.

2 Codevelopment of ENBIOS

Building on works about the semiotic process in modelling (Sebeok and Danesi 2012) and the stages of the modelling process to consider uncertainty (Refsgaard et al. 2007), **Figure 1** shows a framework to explain the co-development process of ENBIOS. The framework includes 3 stages: (i) model definition, (ii) implementation and (iii) feedback, and the steps taken within each of them from the identification of relevant narratives to the design of the structure, the harmonization with energy system model semantics, the set up and the calibration that have been performed prior to the first (alpha) version of the module. The next steps include the actual simulation using the results of the energy models and the evaluation of results, both of which are developed during the last year of SENTINEL. ENBIOS' development has included the advances of WPk s 1 (user needs), 4 (energy system models), 6 (SENTINEL platform) and 8 (Intercomparison protocol).

The energy modellers and decision makers' participation in the development of ENBIOS has reached level three of five (involve) in the spectrum developed by the International Association for Public Participation. Whereas participants external to SENTINEL were mostly involved in the identification of relevant narratives and the structure design (stages 1 and 2), SENTINEL energy modellers helped complete the harmonization and set up (stages 3 to 5).

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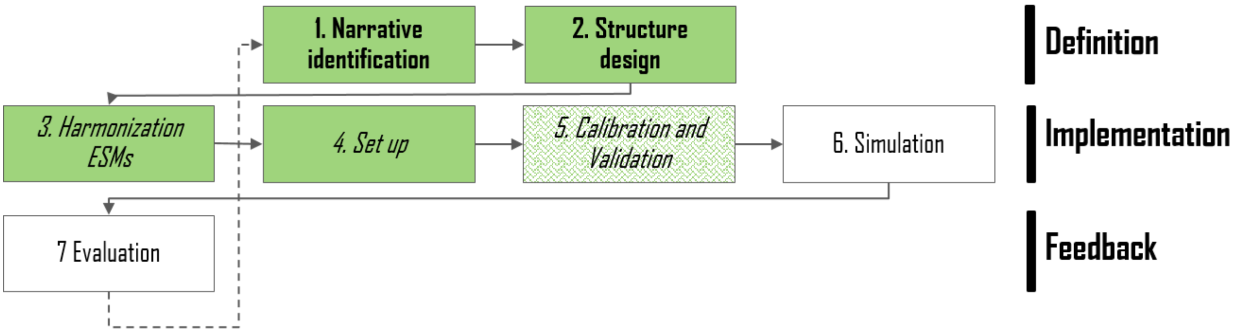
[1] Note that the original name proposed was ENVIRO, which had to be changed to ENBIOS due to the high number of python packages that used the keyword enviro.

Figure 1: Steps of the process followed in the co-development of ENBIOS showing participation of external users (bold) and internal SENTINEL users (italics), completed steps (green) and ongoing steps (shadowed green). Full lines are flows of information and dotted lines represent feedbacks.



2.1 External user needs: defining the internal structure

The work of SENTINEL in the identification of external user needs was developed in work package (WPk) 1 (user needs) and WPk 7 (case studies) and included a series of document analysis, surveys and workshops also involving WPk 3 and WPk 4 of the project. During this process five main environmental concerns were identified (Gaschnig et al. 2020, Madrid-López, C. et al. 2021), which are included in ENBIOS and are covered in table 1.

The work on external user needs developed in WPk 1 identified as general concerns the impacts of the material dependency and supply chain of electricity production; the GHG emissions; and the environmental impacts on biodiversity/land, water and human health. These parameters were used to decide the focus of ENBIOS, the LCA inventory flows included and the impact assessment methods chosen. Although ENBIOS includes a number of LCIA methods, the first tests have been developed using the ReCiPe 2016 midpoint methods (individualist, hierarchical and egalitarian for short-, medium- and long-term impacts) (Huijbregts et al. 2017). Also, for the assessment of the material dependency, a new impact assessment method was created.

Table 1. Summary of external user needs as collected in WPks 1 and 7.

External user need	How ENBIOS provides this information
Inclusion of raw material requirements & circularity	• Identification of main raw material demand • Development of a new indicator of supply risk • Including recycling rates
Consideration of impacts over full life cycle	• Full Life Cycle inventories are passed on to MuSIASEM to perform the environmental impact assessment over the value chain
Inclusion of impacts on biodiversity	• Life cycle impacts assessment (LCIA) methods included assess impacts on biodiversity
Inclusion of more detailed calculations of GHG emissions	• Total GHG emissions are included for CO_2, CH_4 and NO_x • Indicator of Global Warming Potential in CO_2 equivalent
Inclusion of other forms of pollution	• Other indicators of air, land and water pollution (e.g., abiotic depletion, acidification, eutrophication, land and aquatic ecotoxicity)
Inclusion of other factors influencing human health	• Other indicators of human health (e.g., human toxicity potential cancer and non-cancer related)
Inclusion of land & water use	• Indicators of land and water use
Externalization of impacts	• Space to define in each case study if impacts are domestic or imported

The work on case study definition developed in WPk 7 resulted in the definition of two energy carrier production scenarios: the transition scenario and the net zero scenario (Stavrakas et al. 2021). Consequently, ENBIOS focuses on the *production of energy carriers*, namely electricity, heat and fuels, taking the results of the optimized system design generated in WPk 4 of the project. The participants of the Nordic case study also highlighted the relevance of the externalization of environmental impacts related to the import of biomass, for what ENBIOS includes the capability of distinguishing between domestically produced and imported energy carriers.

2.2 Internal user needs: harmonizing with energy models

The integration modelling work in SENTINEL is mostly related to WPks 4 (system design), 6 (SENTINEL platform) and 8 (intercomparison of results). The needs to consider in ENBIOS relate to the semantics of the energy model results; the ENBIOS results data compatibility; the way in which constraints are included in the energy models; the temporal and spatial resolution; and the accessibility to environmental data. They are summarised in Table 2.

Table 2. Summary of internal user needs from WPk s 4, 6 and 8.

Internal needs	How ENBIOS provides this
Compatibility with SENTINEL semantics	• Development of index for friendly_data package to link ENBIOS functionality and the standard data nomenclature within the SENTINEL project
Compatibility with IAMC semantics	• Results structured in IAMC format
Format compatibility	• ENBIOS is a Python package producing .csv formatted outputs
Definition of constraints	• Adding environmental information for each pathway, avoiding normative ranking
Temporal and Spatial Resolution adaptability	• Matching extend and resolution to one year • Capabilities to differentiate regions
Data access to pay walled environmental data	• Translator transforms ecospold data into ENBIOS compatible input

In SENTINEL two different semantics are used respectively for the platform's structuring of the energy system model results and for the intercomparison of results with other models. The platform structuring of the archive follows the semantics set for the friendly_data package[2]. The intercomparison of results is structured following the semantics of the IAMC data format[3]. In each of them, the combination of technologies, primary energy sources and energy carriers is structured differently. The MuSIASEM part of ENBIOS registers the system design (or pathway) given by the energy system models and also must report the results in a way that is compatible for intercomparison, both semantics were considered. The friendly_data package transforms the output of the SENTINEL models into SENTINEL semantics before it is archived in the platform. To be able to use data from the platform an ENBIOS/friendly data dictionary was created that serves also as index to report ENBIOS results to the platform. Additionally, to report the results of ENBIOS in IAMC semantics, an ENBIOS/IAMC dictionary was created.

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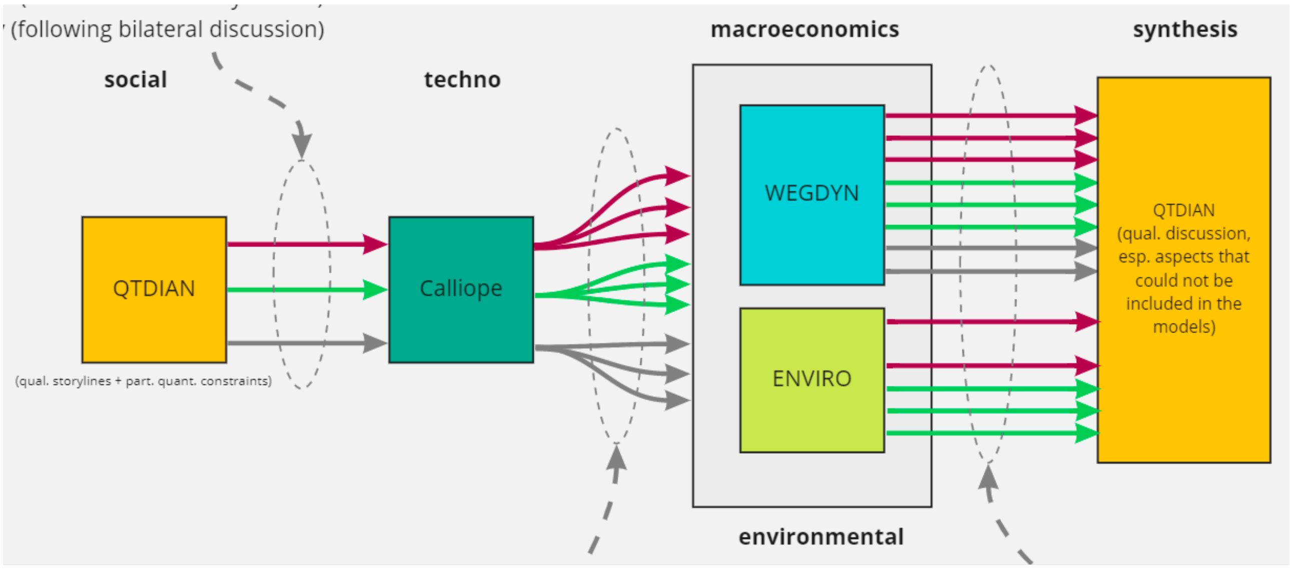
[2] https://github.com/sentinel-energy/friendly_data

[3] https://data.ene.iiasa.ac.at/database/

The models of SENTINEL are written in a variety of languages and mostly take data in text (.csv .txt) format. To make ENBIOS more accessible, the module is written in a dedicated python environment and returns results in .csv format. ENBIOS does not have a user interface yet as the development of the backend was the priority within SENTINEL and most of the expected ENBIOS users were modellers with a fair knowledge of programming. However, a Jupyter notebook has been prepared to make the module more accessible.

Figure 2. Integration of ENBIOS (ENVIRO) in the SENTINEL workflow



The social storylines developed by QTDIAN (REF to Del 2.3) are used within SENTINEL to define social constraints as input parameters for energy models. The resulting ENBIOS indicators, however, cannot be used in the same way without producing a normative ranking of energy pathways, given that the prioritization of environmental aspects is subjective to the decision maker. The three storylines of QTDIAN prioritise people, market and government narratives in the definition of energy model constraints and may also be used in the definition of benchmarks against which the environmental parameters calculated by ENBIOS can be compared. ENBIOS has, therefore, been defined as a simulation tool and not as an optimization tool and its objective is to calculate the environmental and bioeconomic indicators associated to each energy system design. However, the capability of comparing indicators like water use, raw materials or biodiversity loss against an externally defined set of benchmarks is included in ENBIOS. Figure 2 shows how the constraint of pathways works for ENBIOS (ENVIRO).

The temporal and spatial resolution of SENTINEL models range from hours to years and ENBIOS inherits the resolution of the input data. It is recommended to use ENBIOS for a yearly resolution for two reasons. First, because a resolution of hours does not cover the changes in ecosystems, which can be observed only with longer resolutions. And second, because the resolution of the life cycle databases used is annual. However, ENBIOS could, in principle, be used to calculate impacts with shorter resolutions when it is relevant, like in the case of water use when it is compared with the natural seasonal regimes of the Mediterranean water cycle. On the other hand, ENBIOS has the possibility of calculating results for small, medium and longer regions, but for the moment it does not provide a fully regionalised assessment, a feature that we consider for future developments as explained in the methodology section that follows.

Finally, the most important issue that energy models will face is the access to pay walled environmental data, as the best life cycle databases for energy systems (Ecoinvent and GaBi) are both commercially licensed. This is an issue that is difficult to overcome as any environmental modelling tool requires of a complete characterization database. To meet this challenge ENBIOS includes a translator of Ecoinvent and GaBi data format (.spold) to allow license holders to use the module. Also, we consider for the future the development of an internal library of precalculated coefficients that will allow the user with no access to pay walled data to have a rougher estimation of the environmental parameters.

3 Methodological roots

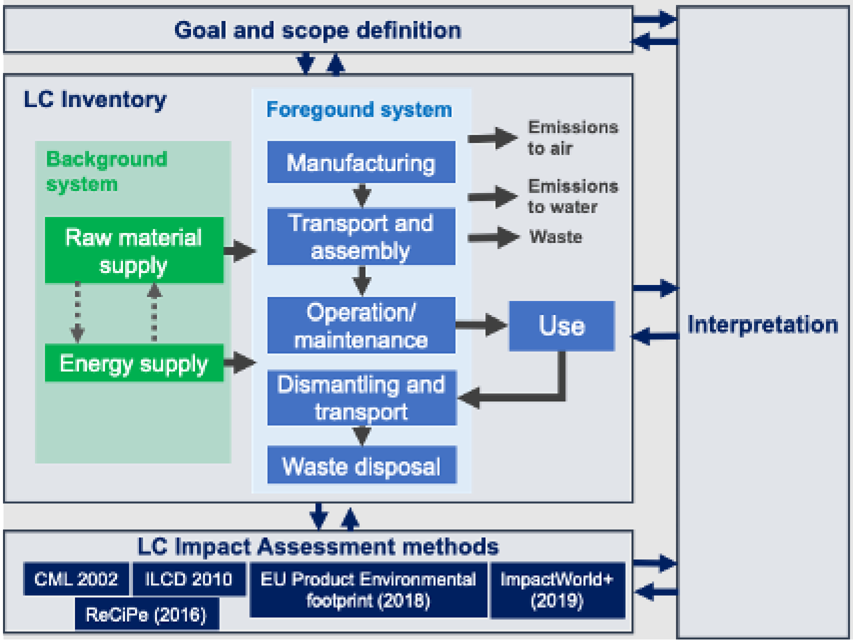
As commented above, ENBIOS' internal engine is powered by two complementary frameworks: Life Cycle Assessment (LCA) and the Multi-Scale Integrated Assessment of Socio-ecosystem metabolism (MuSIASEM).

3.1 Life Cycle Assessment

Life Cycle assessment (LCA) is methodological framework used to evaluate the environmental burden of a product or service by accounting the inflow and outflow of materials and energy, including waste, extracted from or released to the environment (Guinée 2002) through the entire productive chain of a process using a sequential approach. A complete LCA accounts for the inflows and outflows of the system 'from cradle to grave', including extraction of materials, manufacturing, consumption and recycling to the final disposal. LCA can be divided into four steps: 1) goal and scope definition, including functional unit and analytical system boundaries, 2) life cycle inventory (LCI) analysis, 3) life cycle impact analysis (LCIA) and 4) interpretation. A sketch of the implementation of an LCA for energy systems is shown in figure 3.

In LCA, a functional unit is defined, which serves as the quantitative reference for the analysis. For energy systems, this functional unit is usually defined in terms of generation of energy carriers (1 KWh of electricity or 1J of heat, for example) or in installed power capacity (1MW, for example). The main challenges in the definition of a functional unit for the assessment of energy systems, is that typically different stages of the productive chain require a different functional unit. For example, the construction of a power station is better assessed in terms of its material and energy requirements and environmental impacts in terms of MW of installed capacity. Namely, a power station with higher capacity will require more materials and energy to be built than a lower capacity station. However, the operation and generation stages are better assessed in terms of the actual production of energy carriers. This is particularly important for the case of electricity production from fossil fuels in which each KWh produced comes at the cost of a certain amount of GHG emissions among other impacts.

Figure 3. ISO14040 LCA framework (in light blue). Background system (in green colour) and foreground system (in blue colour) included. LCIA methods are illustrated in dark blue rectangles.



The reference of the functional unit is used to generate an inventory with the flows associated to all the processed included in the system boundaries. Flows like raw material, energy, atmospheric emissions, water emissions, solid wastes, and other releases for the entire life cycle of a product, process, or activity are included in the inventory. The inventory has a higher resolution for those flows that form the foreground of the analytical system than for those included in the background system (Guinée et al. 2011). The foreground system refers to the processes under analysis, in our case the energy system design provided by other SENTINEL models. The background system includes the processes that are needed for the supply of the inputs required by the foreground system. Examples of background system generally include the infrastructure processes related to power plants or the fossil fuels production. Generally, inventory data for the foreground system is collected by the analyst whereas the background information is taken from existing databases. Currently, the most complete and widely used databases are Ecoinvent (Wernet et al. 2016) and GaBi (Kupfer et al. 2020).

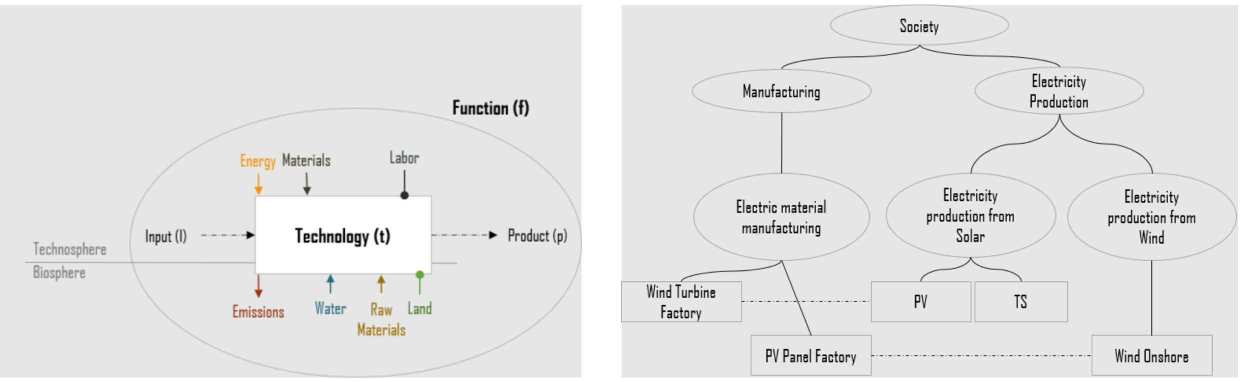
In the Life Cycle Impact Assessment (LCIA) the inventory flows are classified by their contribution to specific environmental impacts and multiplied by characterization factors to calculate the value of those impacts. These steps of classification and characterization result in *midpoint* indicators which can be later normalised, valued and/or ranked to estimate *endpoint* indicators. The type of indicators that is more relevant for an analysis depends on its purpose. The process of valuation and normalization needed for the calculation of endpoint indicators makes them more subjective but commensurable whereas midpoint indicators are non-commensurable with one another but avoid miscalculation of values due to insufficient knowledge to complete the calculation. The calculation of both types of indicators follows established LCIA methods. Some of the methods are single indicator -Cumulative Exergy Demand (Bösch et al. 2007)- whereas others include a list of indicators, like ILCD2010 (Tobergte and Curtis 2013), ReCiPe 2016 (Huijbregts et al. 2017), the EU Product Environmental Footprint 2018 (Sala S. et al. 2019) or Impact World+ (Bulle et al., 2019).

Typically, multi-indicators methods are more generalist and single-indicator methods are most specific for the particular impact studied. For example, water use is included within the battery of a number of multi-indicator methods, however a specific method, AWARE, has been developed for a better assessment of impacts related to water use (Boulay et al. 2018).

3.2 Multi-Scale Integrated Assessment of Socio-ecosystem Metabolism

MuSIASEM (Giampietro et al. 2009) is a methodological framework designed for the sustainability assessment of energy system configurations and based in the study of societal metabolic patterns (Giampietro et al. 2014b) and the flow/fund model (Georgescu-Roegen 1971). It represents societal functions and structures as *processors* organised in a multi-level hierarchy (Di Felice et al. 2019) of *holons* (Koestler 1967), dual nature entities that can be assessed at the same time as a part of a bigger system or as unitary systems on its own as shown in figure 4. Holons and the resulting hierarchical holarchy (Koestler 1967) are represented in MuSIASEM using dendrograms, tree-like schemes where societal functions are connected to others using parenting relations.

Figure 4. Representation of a structural processor (technology t) that contributes to a functional processor (function f) as an individual system (left) and as a part of an energy system design (right) represented in a dendrogram.



MuSIASEM studies three types of relations: intraprocessor, intralevel and interlevel. *Intraprocessor* relations are given by the mix of inputs and outputs, as represented in figure 4 above. Inputs and outputs can come from / go to either the biosphere (another ecosystem process) or the technosphere (another social processor). Intraprocessor relations are assessed in terms of technical coefficients, flow/fund (Georgescu-Roegen 1971) rates, typically in terms of flows per hour of human activity or hectare of land involved in a process (Velasco-Fernández et al. 2018). *Intralevel* relations are those that connect different processors of the same level within the hierarchy and are used to characterise a sequential pathway (Cadillo-Benalcazar et al. 2020). These relations are similar to the relations assessed in LCA in that they consider the full value chain of a process. *Interlevel* relations refer to the connection between a process and its parent/children. Its assessment borrows principles of relational biology to connect whole systems with their components (González-López and Giampietro 2018, Cabello et al. 2019).

These relations are used to characterise the contribution of a certain societal function to the upper levels of the hierarchy and the constraints posed by the upper levels to the lower in terms of material and energy flows. Typically, this characterization is done in terms of trade-offs between the different flows involved in the functioning of the society. Figure 5 shows a MuSIASEM representation of the trade-offs between water, energy and raw materials. The water and raw material supply functions provide, respectively, water and raw materials to the energy system, which, in turns, provides energy to the water and raw material functions. The resulting trade-offs are hierarchically organised in *supply and end use matrices* that are crosschecked to

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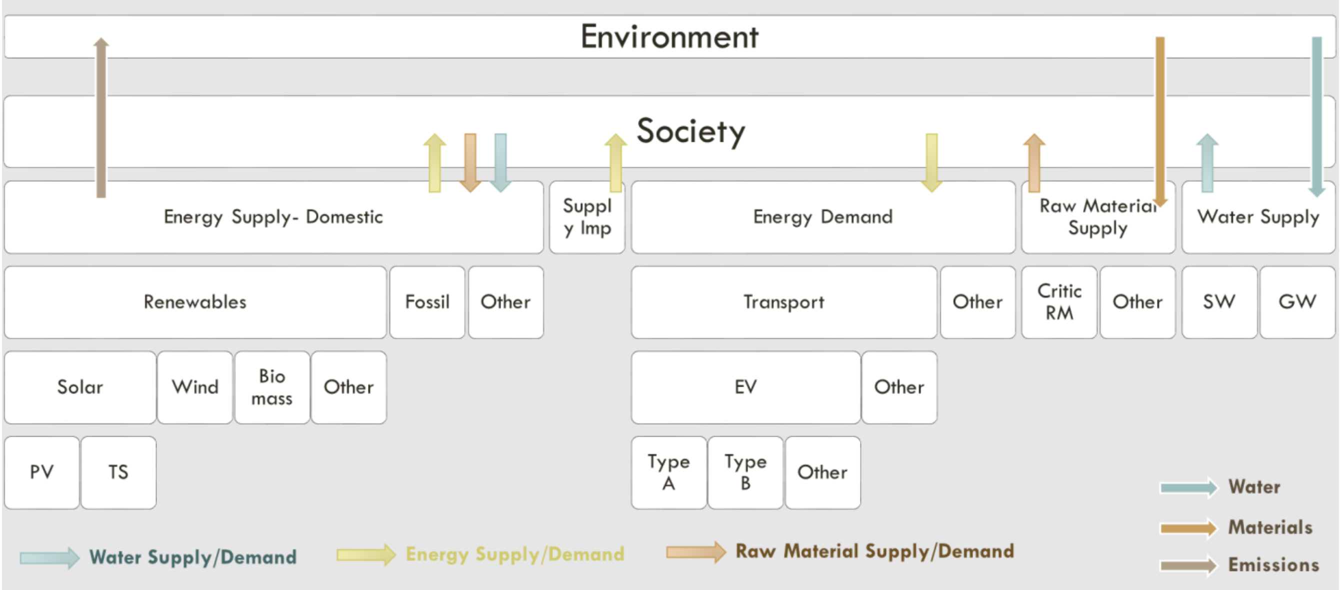
identify the main constraints of the metabolic system (Pérez-Sánchez et al. 2019). Typically, indicators included in the supply and end use matrixes are mostly related to energy, water, agricultural and monetary flows as well as human activity, defined as the amount of hours devoted to a societal function, and land use.

Figure 5. Example of the hierarchical representation of trade-offs in MuSIASEM.



The environment is represented in MuSIASEM as a level above the society in the hierarchy and environmental impacts are assessed using a different narrative (Madrid et al. 2013) and a different battery of indicators mostly related to the depletion of natural resources (Ripa et al. 2021). The relation between pressures and actual impacts has been covered in MuSIASEM tangentially only in the assessment of agricultural systems (Madrid-López et al. 2014, Renner et al. 2020).

For the calculation of the technical factors that characterise the intraprocessor mix, and the supply, end use and environmental pressure matrices, MuSIASEM relies in data from different sources. Technical coefficients at the processor level are often gathered from LCA databases (Di Felice et al. 2018, Ripa et al. 2021), literature or technical reports (Diaz-Maurin and Giampietro 2013), and statistical databases (Velasco-Fernández et al. 2015).

3.3 Connecting LCA and MuSIASEM

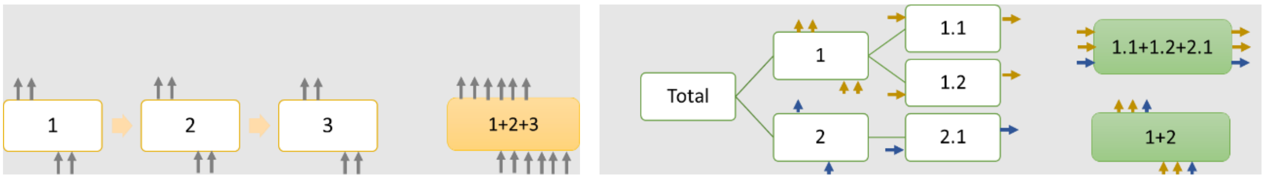
As figure 6 shows, MuSIASEM and LCA represent energy systems differently. However, they have some features that makes them synergic. The integration of MuSIASEM and LCA in ENBIOS has been done taking into account the following aspects:

- MuSIASEM uses flow/fund technical coefficients to characterise processes (societal functions) and their interlevel and sequential relations. The recognition of these sequential pathways is the point of connection with the LCA framework. In this way MuSIASEM can be used to upscale the results of an

LCA to the full system. To do this, it is necessary to allocate LCA processes (technologies) to MuSIASEM processes.

- If MuSIASEM and LCA share the sequential representation of a system and, consequently, both use LCA inventories as data sources, an upscaling of those sequential pathways can complement and improve both the bioeconomic and environmental assessments performed in MuSIASEM.
- Current LCIA methods might not recognise the trade-off assessment capabilities of MuSIASEM and consequently new impact assessment methods for MuSIASEM might have to be created.

Figure 6. The two approaches in the representation of the analytical system: LCA (left) and MuSIASEM (right)

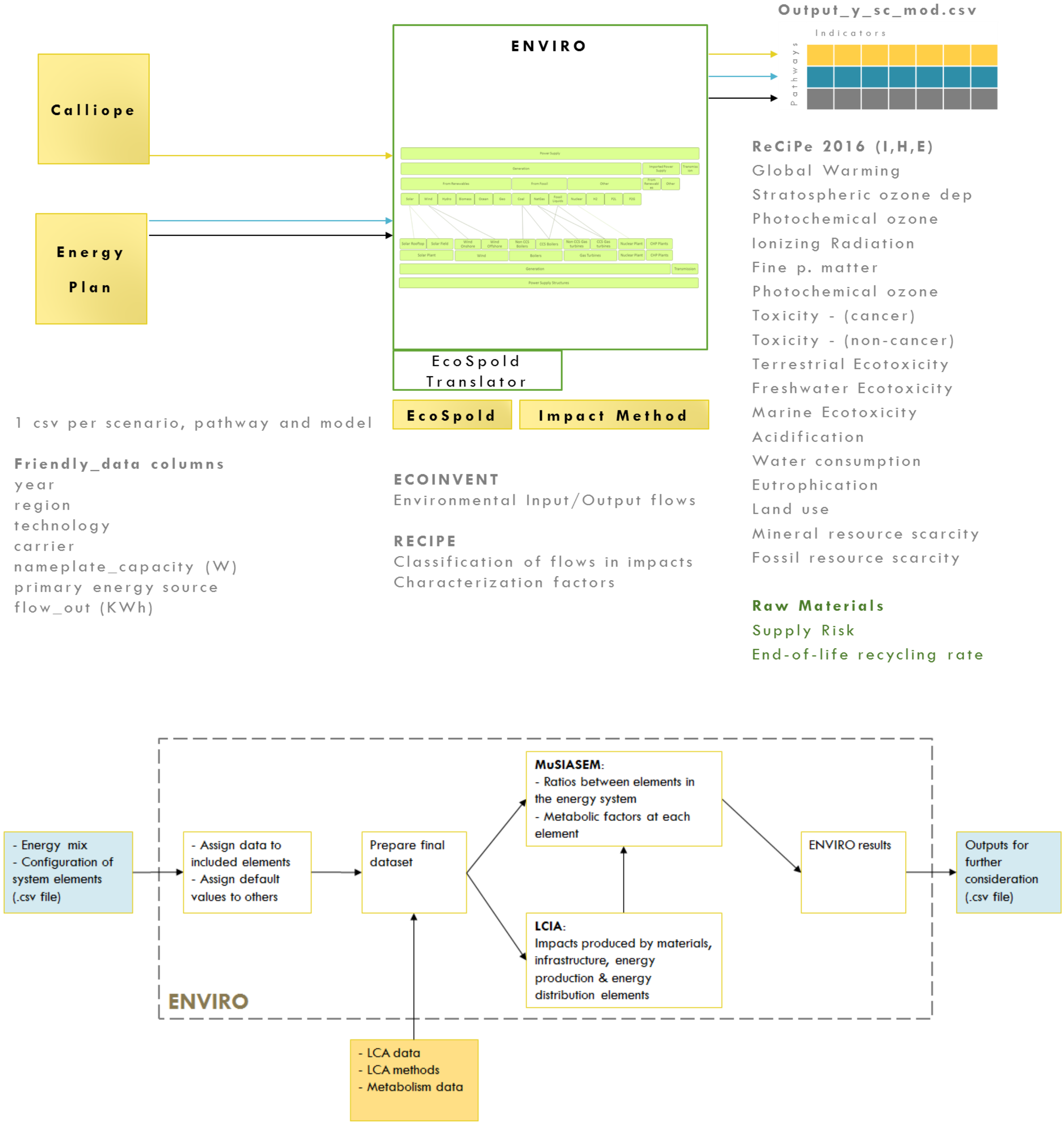


4 ENBIOS framework: Architecture

4.1 What is ENBIOS

ENBIOS is an assessment framework created to integrate the life cycle and systemic environmental impacts and bioeconomic constraints of energy system configurations. As previously commented, after evaluating the internal and external user needs, ENBIOS has been defined as a simulation framework and not an optimization one. Its development into a software system is described in section 5.

Figure 7. Summary of the architecture of the ENBIOS framework (above) and its workflow (below)



ENBIOS derives a set of specific biophysical (water, materials, etc.) extractions and emissions to be derived for each energy source within a system. Being ENBIOS part of the SENTINEL platform. The structure of the system is given by the energy optimised transition pathways developed by SENTINEL energy models like Calliope or Energy Plan for each of the two scenarios (transition and net zero) and three storylines (market, government and people – oriented) considered in the project. The framework is summarised in figure 7.

4.2 Data inputs

ENBIOS requires a significant amount of information to be compiled and integrated. Nevertheless, once the framework of the system and the basic system information has been defined, simulations for different scenarios can be undertaken by making minor changes to system configurations and energy data quantities. The structural and data components required to successfully set-up and complete a simulation run in ENBIOS are divided into two general categories:

- General system setup
- Life cycle assessment data and methods
    - Defining new raw material related methods

These will each be discussed in the sections that follow.

4.2.1.1 Life cycle impact assessment (LCIA) methods ReCiPe 2016)

As explained above, an LCIA method is a specification that defines the way in which the individual inventory information within the LCI dataset is converted into data for specific impact categories and each method is based on different classification and characterization factors. A number of multi-indicator methods are included in the ENBIOS method library, from which the analyst can choose the most appropriate for their analysis. Table 3 summarises the methods that are included in the library.

Table 3. Summary of the methods included in the ENBIOS method library. Note that 'LT' is an abbreviation of 'long term' - methods that do not include it do not consider impacts that occur more than 100 years after the activities within the process have been completed

CML 2001 (superseded)	EDIP2003 w/o LT	ReCiPe Endpoint (H,A)
CML 2001 w/o LT (superseded)	EDIP2003	ReCiPe Endpoint (I,A)
cumulative energy demand	EF1.0.8 midpoint (superseded)	ReCiPe Midpoint (E) V1.13 no LT
cumulative exergy demand	EF1.0.8 midpoint no LT (superseded)	ReCiPe Midpoint (E) V1.13
eco-indicator 99, (E,E) (superseded)	EF2.0 midpoint no LT	ReCiPe Midpoint (E) w/o LT
eco-indicator 99, (E,E) w/o LT (superseded)	EF2.0 midpoint	ReCiPe Midpoint (E)
eco-indicator 99, (H,A) (superseded)	EPS 2000	ReCiPe Midpoint (H) V1.13 no LT
eco-indicator 99, (H,A) w/o LT (superseded)	IMPACT 2002+ (Endpoint)	ReCiPe Midpoint (H) V1.13
eco-indicator 99, (I,I) (superseded)	IMPACT 2002+ (Midpoint)	ReCiPe Midpoint (H) w/o LT
ecological footprint	IPCC 2001 (superseded)	ReCiPe Midpoint (H)
ecological scarcity 1997 superseded)	IPCC 2007 (superseded)	ReCiPe Midpoint (I) V1.13
ecological scarcity 2006 (superseded)	IPCC 2007 no LT (superseded)	ReCiPe Midpoint (I)
ecological scarcity 2013 no LT	IPCC 2013 no LT	selected LCI results, additional
ecological scarcity 2013	IPCC 2013	selected LCI results
ecosystem damage potential	ReCiPe Endpoint (E,A) w/o LT	TRACI
EDIP (superseded)	ReCiPe Endpoint (E,A)	USEtox w/o LT
EDIP w/o LT (superseded)	ReCiPe Endpoint (H,A) w/o LT	USEtox

The internal tests of ENBIOS were developing using the multi-indicator ReCiPe2016 H method (Huijbregts et al. 2017). A summary of the outputs available using this method is provided in Table 4 as a sample of the type of results that multi-indicator methods can provide.

Figure 8. Summary dendrogram for Power Supply Branch. Left side are functions and right side are structures. Note that the use of carbon capture and storage (CCS) functionality for turbines and combined heat and power (CHP) thermal plants is not currently supported, but may be included as the module develops, subject to the availability of suitable LCA data for CCS infrastructure

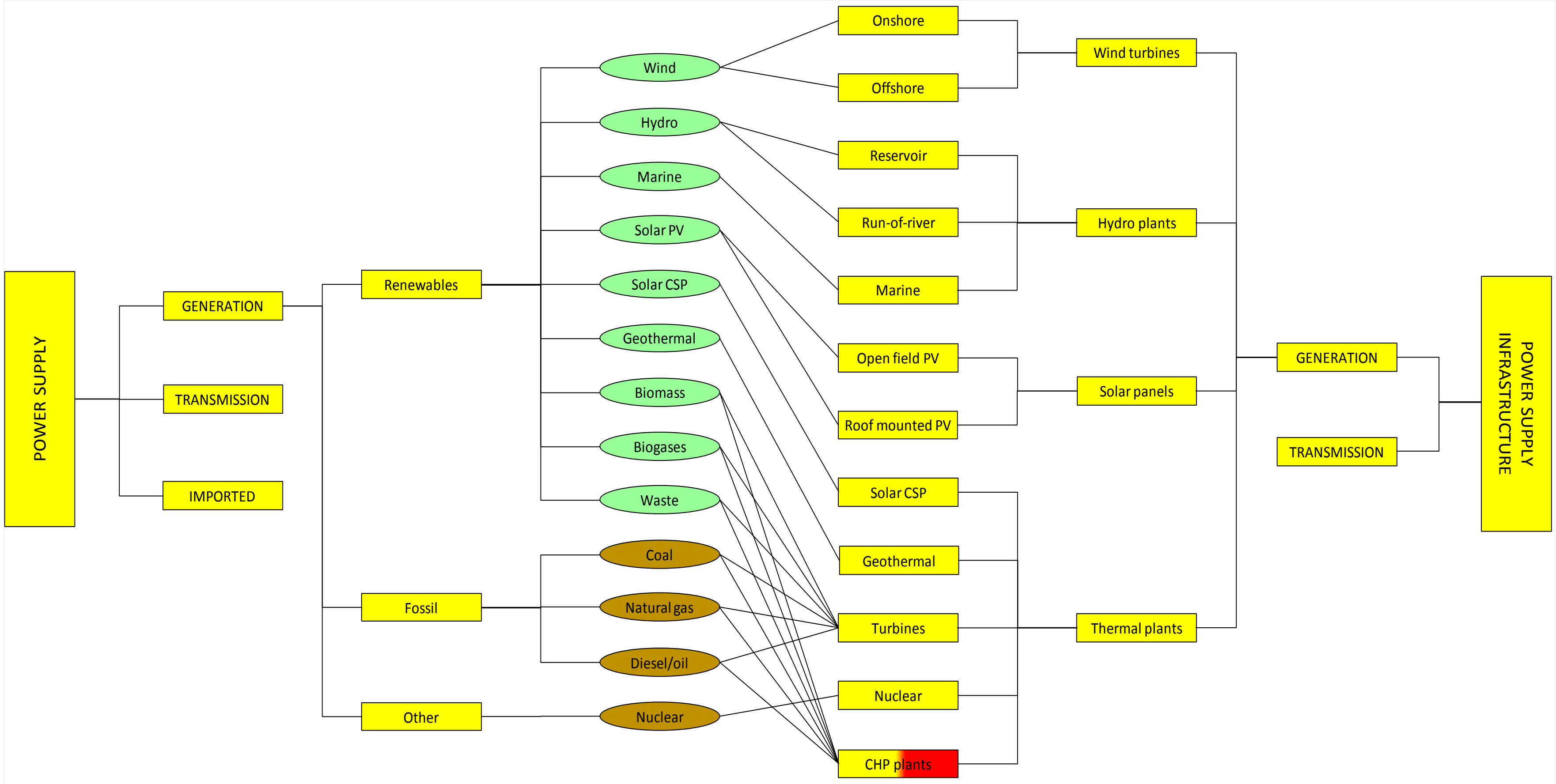


Table 4. Summary of output indicators available using ReCiPe 2016 LCIA method (Huijbregts et al. 2017).

Indicator	Description
ALOP	agricultural land occupation
GWP500	climate change (global warming potential)
FDP	fossil depletion
$FETP_{inf}$	freshwater ecotoxicity
FEP	freshwater eutrophication
HTP_{inf}	human toxicity
IRP_HE	ionising radiation
$METP_{inf}$	marine ecotoxicity
MEP	marine eutrophication
MDP	metal depletion
NLTP	natural land transformation
ODP_{inf}	ozone depletion
PMFP	particulate matter formation
POFP	photochemical oxidant formation
TAP_{500}	terrestrial acidification
$TETP_{inf}$	terrestrial ecotoxicity
ULOP	urban land occupation
WDP	water depletion

4.2.2 New impact assessment methods

As mentioned above, even though the library of LCIA methods is extensive, there is still potential for creating improve methods for the assessment of particular indicators. This is the case for raw materials, for which the closest ReCiPe indicator, metal depletion, is not robust enough to inform policies about the material dependency of energy systems. For ENBIOS two new raw material-related methods were created and are summarised below.

4.2.2.1 The circularity of energy technologies in the EU

The end-of-life recycling input rate (EoL-RIR) reflects the total material input into the production stage that comes from the recycling of post-consumer scrap and is regarded as a robust measure of recycling’s contribution to meeting materials demand. The Eurostat database uses the EOL-RIR parameter as an indicator for monitoring the EU’s progress towards a circular economy on the thematic area of 'secondary raw materials' and the current paper proposes the use of EOL-RIR as a way of monitoring circularity aspects of energy systems within ESM studies. The EoL-RIR for a technology can be calculated by considering the EoL-RIR of individual materials (European Commission 2020) in relation to the overall mass of materials in the item of infrastructure under study. In the case of ENBIOS, a composite value of EoL-RIR is calculated using the 55 critical raw materials (CRMs) defined by the EC that also have listings within the LCI inventory data provided in the Ecoinvent database.

As the EoL-RIR rates defined for these materials are expressed as a percentage, the summation of the final EoL-RIR for each process must be divided by the total mass of all materials to provide the final EoL-RIR value. Accordingly, the final formula is as follows:

$$EoL - RIR_{technology} = \frac{\sum_{i=1}^{n} m_i \; EOL - RIR_i}{\sum_{i=1}^{m} m_i}$$

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 837089.

where:
$EoL - RIR_{technology}$ = net EoL-RIR of the technology under study [%]
n = number of individual materials in the technology under study
m_i = mass of material i contained in the technology under study [kg/energy or power unit]
$EoL - RIR_i$ = EoL-RIR of material i [%]

The results will provide a better understanding of the circularity of a technology from a material perspective. To assess the circularity of the technology itself, further analysis that assesses the disassembly along with a more detailed analysis of the material recovery from these technologies would need to be further developed.

4.2.2.2 *The supply risk of energy technologies in the EU*

The key output from the EU's 2020 critical raw material (CRM) assessment (European Commission 2020) was the supply risk (SR) factor that quantifies the overall SR for each material as a dimensionless constant based on a number of physical and geopolitical factors. This parameter also represents a key aspect of the ENBIOS module as the large-scale deployment of new energy technologies, and renewable energy in particular, could prove to be less feasible if the materials required to build the necessary infrastructure are scarce or difficult to obtain.

Initial attempts to define a methodology for creating a composite SR score were based on a simple pro-rata approach. However, in order to capture the importance of materials that exist in much smaller quantities, an additional parameter was required to normalise the amounts of required materials using some measure of overall abundance of supply. Consequently, in the final formula, each material intensity value must first be normalised by dividing it by the annual consumption level within the EU. This provides a more useful measure of the significance of using the given amount in relation to the overall supply. The proposed formula, which also utilises the 55 CRMs identified by the EC for which LCI data is available, is as follows:

$$SR_{technology} = \sum_{i=1}^{n} \frac{m_i \, SR_i}{c_i}$$

where:

$SR_{technology}$ = net SR of the technology under study [yr/energy unit]
n = number of individual materials in the technology under study
m_i = mass of material i required for process [kg/energy unit]
SR_i = SR of material i [dimensionless]
c_i = annual consumption level in EU of material i [kg/yr]

It is noted that, although the final value of SR is essentially dimensionless, the final units are actually the timeframe of the consumption data divided by the unit that the material intensity is based upon. For example, for one MJ of electricity produced, the final units would be, in fact, the relatively meaningless year per MJ. However, assuming calculations are based on material intensity data that uses the same units, all final values of SR can be directly compared.

4.3 Results

As mentioned in section 2, SENTINEL's work on intercomparison of results is organised around the IAMC data format. This hierarchical standard is designed to organise information on energy supply, demand, transmission and storage but it does not have a proposal to name environmental impacts beyond GHG emissions. Consequently, a new standard for the inclusion of LCIA indicators with MuSIASEM structure in the IAMC nomenclature had to be defined together with WPk 8. The resulting ENBIOS IAMC Standard for environmental impacts is summarised in table xx.

Table 5.ENBIOS IAMC standard for environmental impacts of energy systems

imp	**ReCiPe H**	**Global Warming**
		Stratospheric ozone depletion
		Photochemical ozone
		Ionizing Radiation
		Fine p. matter
		Toxicity - (cancer)
		Toxicity - (non-cancer)
		Terrestrial Ecotoxicity
		Freshwater Ecotoxicity
		Marine Ecotoxicity
		Acidification
		Water consumption
		Eutrophication
		Land use
		Mineral resource scarcity
		Fossil resource scarcity
	Raw Material	Supply risk
		End-of-life recycling rate
inv	Emissions to air	CO2
		CH4
		NOx
	Emissions to soil	a
		b
		c
	Emissions to water	To River
		To Aquifer
		To Sea
	Resource Use	Water
		Land
		Biomass
	Raw materials	a
		b
		c

The general label for this standard is: "enbios_[framework]_[stage]_[method]_[indicator]" that includes the framework used to calculate the indicators ("lca" for life cycle assessment or "met" for metabolism assessment), the stage of the results ("inv" for flows and "imp" for impacts), the impact assessment method used ("recipe" for example), and the indicator (such as "co2", "ch4", "gwp" for global warming potential).

The results are given in the form of a table that contains the chosen impact indicators for each of the functions included in the dendrogram at each of the levels. Table xx shows the head of a sample results file.

Table 6. Head of the resulting .csv file from ENBIOS

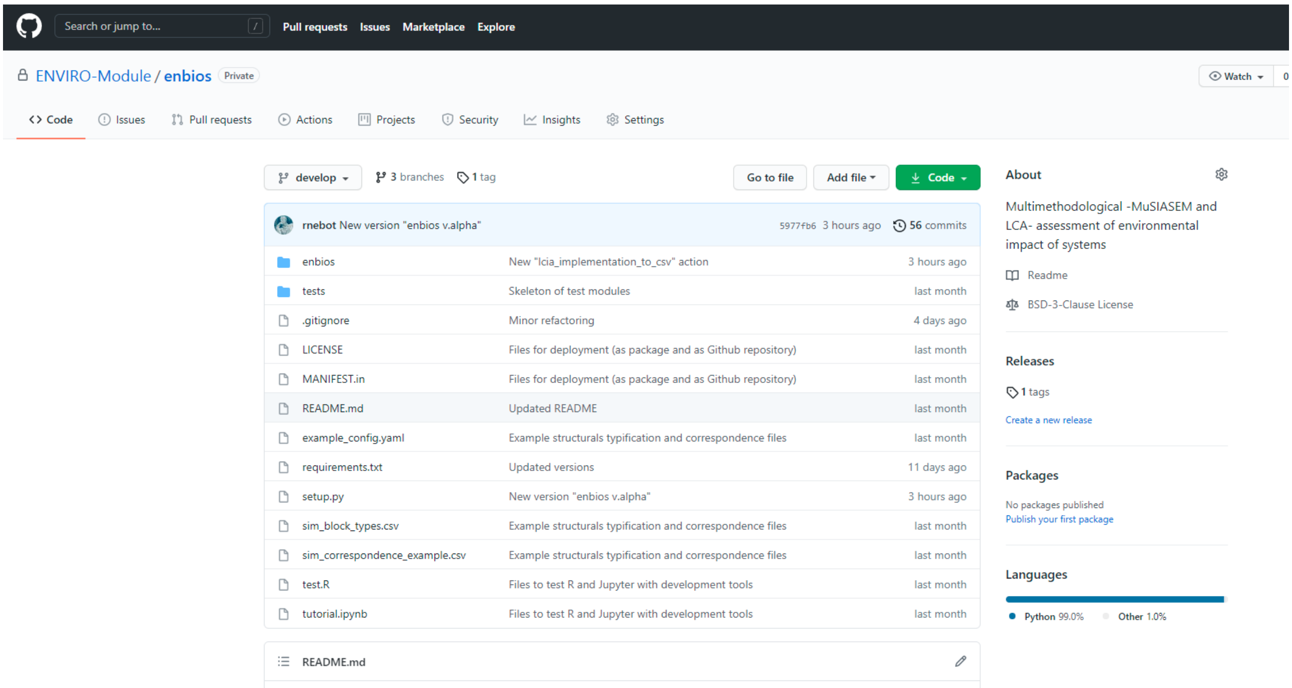
Scenario	Period	Scope	Processor	Indicator	Value
s1	2038	Internal	alb_environment	SR2	2.00E-06
s1	2038	Internal	energy_system	SR2	3.67E-10
s1	2038	Internal	energy_system.electricity_supply	SR2	3.67E-10
s1	2038	Internal	energy_system.electricity_supply.electricity_generation	SR2	3.67E-10
s1	2038	Internal	energy_system.electricity_supply.electricity_generation.electricity_renewables	SR2	3.67E-10
s1	2038	Internal	energy_system.electricity_supply.electricity_generation.electricity_renewables.electricity_wind	SR2	3.67E-10
s1	2038	Internal	energy_system.electricity_supply.electricity_generation.electricity_renewables.electricity_wind.electricity_wind_onshore	SR2	3.67E-10
s1	2038	Internal	energy_system.electricity_supply.electricity_generation.electricity_renewables.electricity_wind.electricity_wind_onshore.ac_ohl_mountain_transmission_alb	SR2	6.34E-12

5 Software description and location

ENBIOS has been developed into an open-source python package and for this deliverable the alpha version is completed. More information can be found in the quick start guide and the user manual in the annexes.

The software repository can be found on github and it is, for the moment, private until the calibration and evaluation stages are completed using the SENTINEL case studies. Figure 9 shows a snapshot of the repository.

Figure 9. Snapshot of the ENBIOS repository on Github



ENVIRO-Module / enbios Private

rnebot New version "enbios v.alpha" 5977fb6 3 hours ago 56 commits

enbios	New "lcia_implementation_to_csv" action	3 hours ago
tests	Skeleton of test modules	last month
.gitignore	Minor refactoring	4 days ago
LICENSE	Files for deployment (as package and as Github repository)	last month
MANIFEST.in	Files for deployment (as package and as Github repository)	last month
README.md	Updated README	last month
example_config.yaml	Example structurals typification and correspondence files	last month
requirements.txt	Updated versions	11 days ago
setup.py	New version "enbios v.alpha"	3 hours ago
sim_block_types.csv	Example structurals typification and correspondence files	last month
sim_correspondence_example.csv	Example structurals typification and correspondence files	last month
test.R	Files to test R and Jupyter with development tools	last month
tutorial.ipynb	Files to test R and Jupyter with development tools	last month

About

Multimethodological -MuSIASEM and LCA- assessment of environmental impact of systems

Readme

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Releases

1 tags

Create a new release

Packages

No packages published
Publish your first package

Languages

Python 99.0% Other 1.0%

6 References

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ANNEX I. ENBIOS Quick Start Guide v.0

1 Introduction

ENBIOS is a software for the environmental and biophysical analysis of energy systems. It computes the relation between energy provision functions within a society and the technologies that provide them, integrating two methodological frameworks: life cycle assessment (LCA) and the Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM).

Once the required structural and data inputs are integrated into an ENBIOS simulation, the software allows a set of specific biophysical extractions and emissions to be derived for each energy source within a system. The structure of the system can then be used within a MuSIASEM framework (known as a ‘dendrogram’) to elaborate indicators that can manipulated to provide a deeper understanding of the inner functions of the system at various levels. This, in turn, allows the user to assess and compare the consequences that relate to the various elements within an energy system in a way that allows a better understanding and method of comparison for a range of future climate policy scenarios.

While the core idea behind ENBIOS is relatively simple, implementing a model simulation requires a significant amount of information to be compiled and integrated before the software can be executed. Nevertheless, once the framework of the system and the basic system information has been defined, simulations for different scenarios can be undertaken by making minor changes to system configurations and energy data quantities.

The following sections provide a concise description of the requirements for operating the software. Firstly, a brief description of the method for installing the software to a local device is provided. The required data inputs are then divided into four categories and discussed in turn. Finally, the method for executing individual simulations and the results that are produced are outlined.

2 Installation

To install ENBIOS, complete the following steps:

Step	**Code**
Install a Python (CPython) >=3.7 runtime. Anaconda3 is recommended: https://docs.anaconda.com/anaconda/install/	
Create a Python virtual environment	`conda create -n enbios_env python==3.7`
Install ENBIOS	`pip install enbios`
Install pycurl	`conda install -c anaconda pycurl`

Once installed, an ENBIOS command should be available from the command prompt (CMD in Windows, Shell in Linux, Terminal in macOS). Simply executing this command without parameters (i.e., entering `enbios`) should produce a summary of the different actions. Here, the main action is ENVIRO; other actions within ENBIOS have the purpose of helping in the construction of inputs, as discussed in the following section.

3 File locations

The software is designed to enable cooperative work on case studies by aligning with existing tools that provide collaborative functionality. When used as a Python package (not discussed in this document), using shared Python or R (rpy2 package) scripts or Jupyter notebooks is possible. However, perhaps a simpler way to collaboratively apply the software is via the use of shared Google Drive locations when operating ENBIOS from a command line.

It is recommended that certain files common to the group working on a case study are placed in a shared folder on Google Drive (other file sharing systems under study). These files are:

- The 'Base' workbook .xlsx (or Google Sheets format) file that defines the energy system structure and general model characteristics
- The .xlsx (or Google Sheets format) file that defines the life cycle impact assessment (LCIA) methods
- The processed workbook file that contains life cycle inventory (LCI) data for the system

All other input files should be located on local computers.

4 Preparation of inputs

The structural and data components required to successfully set-up and complete a simulation run in ENBIOS are divided into three general categories:

- General system setup
- Life cycle assessment data and methods
- System data for individual scenarios

Details of the required inputs within these three categories are as follows:

Feature	**Command(s)**	**Source**	**Comment**
Processors (MuSIASEM dendrogram)	'BareProcessors top levels'	Manually transcribed from graphical dendrogram	Hierarchical schema of the energy sector
InterfaceTypes (MuSIASEM)	'InterfaceTypes'		Types of biophysical flows between processors
Raw material factors	'Parameters Raw Materials'	Data manually written into workbook	
Scalar indicators	'ScalarIndicators'	Non-LCIA indicators are manually specified from the outcome of analytical process	Indicators attached to each structural processor
Provenance references	'RefProvenance'	Manually	Useful to annotate the sources used in interface values
Geographic references	'RefGeographic'	Manually	Useful to annotate location of processors using NUTS codes
LCI database	File location in 'ImportCommands LCI structurals'. File contains information relating to: 'InterfaceTypes',	Workbook generated by `lci_to_nis`	A database of LCI activities used to provide raw LCI information to individual structural processors

Feature	Command(s)	Source	Comment
	'BareProcessors top levels' and 'Interfaces'		
LCIA ReCiPe methods	'DatasetDef', 'LCIAMethods', 'ScalarIndicators'	ReCiPe.xlsx -> `enbios recipe_to_csv` -> recipe2016.csv	
Energy 'mix' at structural processors	'BareProcessors simulation'	Use results from `sentinel_to_nis`. 'Processor' categories and data from SENTINEL outputs should be aligned to the structural processors in 'BareProcessors top levels' using the 'Parent Processor' column	Provides integration between SENTINEL simulation results and MuSIASEM and LCA functions in ENVIRO

5 Execution

Execution of an ENBIOS simulation requires the `ENBIOS` sub-routine to be called, followed by the reference to a configuration file in .yaml format and allows for several driving flags to be specified, as follows:

Execution code
`enbios  /home/enbios/ cfg_file_path.yaml --flags`

.yaml configuration file contents	Description
`nis_file_location`	The URL of the 'Base' workbook file
`correspondence_files_path`	Currently not used. Could be used to define the path of a .csv file in which a mapping from technologies to .spold files and from technologies to the MuSIASEM dendrogram could be specified
`simulation_type`	States the file format of the simulation input. For now, should always be 'sentinel'
`simulation_files_path`	Path to the reference file or folder needed by the specific simulation output format. In the case of 'sentinel', it should be the path of the index .json file used by the 'friendly_data' package to drive the reading of the simulation results
`output_directory`	Path of the local directory where all outputs of the execution will be placed

Flag parameters	**Description**
`just_one_fragment`	If 'True', only the first fragment of the split simulation data will be processed. This reduces simulation time and is useful for troubleshooting. 'False' by default
`generate_nis_base_url`	Because the 'Base' framework model can be quite large, it is possible to have specification issues. If this parameter is set to 'True', a workbook in NIS format is generated returning information on how NIS interprets 'Base'. 'False' by default
`generate_nis_fragment_file`	If 'True', for each fragment the dynamically generated NIS file is written to the output directory. 'False' by default
`generate_indicators`	If 'True', a separate indicators.csv file is written for each of the fragments (the aggregate indicators .csv file is always generated). 'False' by default
`max_lci_interfaces`	If >0, when LCI interfaces are merged into simulation processors, the number of interfaces cannot exceed this parameter. This is useful when checking the system prior to a full execution. By default, this is set to 0, meaning all interfaces are activated

6 Output

The main output of the process is an 'indicators.csv' file which details the indicator results for each defined processor. The file contains the following columns:

Result	Description
`scenario`	To which scenario, coincident with SENTINEL scenario codes, do the indicator values apply
`period`	As above, but relating to time period
`scope`	Scope of the indicator. Can be 'Local' (domestic), 'External' (imports/exports) or 'Total'. Currently only 'Local makes sense'; other rows can be filtered out
`processor`	The processors to which the indicator applies
`indicator`	Name of the indicator
`value`	Value of the indicator

Note that there is currently no 'Region' column, although this could be added in the future, if required.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 837089.

ANNEX II. ENBIOS User Manual v.0

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 837089.

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1 Introduction

ENBIOS is a software system developed within the EU Horizon 2020 project known as SENTINEL that aims to provide support in analysing the effects and impacts of the techno-economic sectors of society on its supporting substrates, i.e., environment and, again, society. The coding was initially based on a previously developed set of software tools known as the Nexus Information System (NIS) developed as part of the Magic Nexus project (Magic Nexus, n.d.; Nebot Medina et al., 2020)

The purpose of ENBIOS is to compute a set of environmental impact and sustainability indicators by building a module that relates the various sources of energy within a system to the pressures caused by the technologies that provide them, integrating information and knowledge from three methodologies: life cycle assessment (LCA), the Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM) method and the dynamic simulation-optimisation of energy networks.

Once the required structural and data inputs are integrated into an ENBIOS simulation, the software allows a set of specific biophysical extractions and emissions to be derived for each energy source within a system. The structure of the system can then be used within a MuSIASEM framework (known as a 'dendrogram') to elaborate indicators that can manipulated to provide a deeper understanding of the inner functions of the system at various levels. This, in turn, allows the user to assess and compare the consequences that relate to the various elements within an energy system in a way that allows a better understanding and method of comparison for a range of future climate policy scenarios. The software is to be employed within the SENTINEL project to analyse different future energy scenarios, particularly those that relate to the transition towards higher levels of renewable energy use.

While the core idea behind ENBIOS is relatively simple, implementing a model simulation requires a significant amount of information to be compiled and integrated before the software can be executed. Nevertheless, once the framework of the system and the basic system information has been defined, simulations for different scenarios can be undertaken by making minor changes to system configurations and energy data quantities.

The following sections provide a concise description of the requirements for operating the software. Firstly, a brief description of the method for installing the software to a local device is provided. The required data inputs are then divided into three categories and discussed in turn. Finally, the method for executing individual simulations and the results that are produced are outlined.

2 Installation of software

To install ENBIOS, complete the following steps:

- Install a Python (CPython) >=3.7 runtime. Anaconda3 is recommended: (https://docs.anaconda.com/anaconda/install/)
- Create a Python virtual environment:

```
conda create -n enbios_env python==3.7
```

- Install ENBIOS:

```
pip install enbios
```

- Install pycurl:

```
conda install -c anaconda pycurl
```

Once installed, an ENBIOS command should be available from the command prompt (CMD in Windows, Shell in Linux, Terminal in macOS). Simply executing this command without parameters (i.e., entering enbios) should produce a summary of the different actions. Here, the main action is ENVIRO; other actions within ENBIOS have the purpose of helping in the construction of inputs, as discussed in the following section.

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3 Preparation of inputs

The structural and data components required to successfully set-up and complete a simulation run in ENBIOS are divided into three general categories:

- General system setup
- Life cycle assessment data and methods
- System data for individual scenarios

These will each be discussed in the sections that follow.

The software is designed to enable cooperative work on case studies by aligning with existing tools that provide collaborative functionality. When used as a Python package (not discussed in this document), using shared Python or R (rpy2 package) scripts or Jupyter notebooks is possible. However, perhaps a simpler way to collaboratively apply the software is via the use of shared Google Drive locations when operating ENBIOS actions from a command line.

It is recommended that certain files common to the group working on a case study are placed in a shared folder on Google Drive (other file sharing systems under study). These files are:

- The 'Base' workbook .xlsx (or Google Sheets format) file that defines the energy system structure and general model characteristics
- The .xlsx (or Google Sheets format) file that defines the life cycle impact assessment (LCIA) methods
- The processed workbook file that contains life cycle inventory (LCI) data for the system

All other input files should be located on local computers.

3.1 General system setup

When creating or altering ENBIOS simulations, the 'Base' workbook file–an Excel (.xlsx) or Google Sheets format file that contains several sheets that define the key aspects of the system–acts as the central 'mothership' for the setup and operation of module simulations. An example of such a file can be found here. The definitions within this file largely follow the approach and nomenclature defined by the previous NIS software package.

3.1.1 Energy system schema

The most fundamental data input to the module is the definition of the energy system schema (i.e., the hierarchical categorisation or framework of the system in question). Indeed, all other data inputs and simulation calculations are ultimately based on the way in which the elements of the system are specified within this hierarchical definition.

The system is defined using the approach defined by MuSIASEM (Giampietro et al., 2009) whereby a system is defined by a 'dendrogram' made up of a collection of elemental nodes known as 'processors'. Although the term is defined in more detail elsewhere (e.g., see (di Felice et al., 2019; González-López and Giampietro, 2018)), a processor essentially represents a single process that can be further defined as being either 'functional' or 'structural' in nature. Structural processors represent the most disaggregated level of the system. Here, a given technology performs a set of biophysical transformations to produce a profile of inputs and outputs for the given structural element. Meanwhile, functional processors are essentially locations where data from structural and other functional processors are aggregated and where further data for the metabolism of inputs to produce outputs can be obtained. To provide an energy-related example, one could define a series of structural processors for electricity produced from wind, solar, hydro and so on; all of these could then be aggregated in a functional processor at the previous level for electricity from renewable sources. Another structural processor at the previous level from this processor could aggregate all of the electricity produced from renewable and non-renewable sources. This approach is highly flexible and can be used to characterise almost any socio-metabolic system that can be defined into a hierarchical framework.

The energy system schema is defined within the 'BareProcessors top levels' sheet of the 'Base' workbook file. The columns that define this are as follows:

- 'Processor' – The name of the processor
- 'ParentProcessor' – The processor, located one level above, where the data from this processor is aggregated
- 'SubsystemType' – Type of subsystem that the processor is within, typically 'Local'
- 'FunctionalOrStructural' – Whether the processor is functional or structural
- 'Accounted' – Turns accounting on ('Yes') or off ('No') for this processor, typically left on ('Yes')
- 'Level' – The level of the processor within the hierarchy. The highest level, for the system as a whole, is set to 'n' and subsequent sub-levels are defined as 'n-1', 'n-2', 'n-3' and so on

3.1.2 Other setup data

The 'Base' workbook file is also the location for defining other general setup data. The majority of this information this will not be discussed in this document and, indeed, will not change from case to case once they have been initially specified. Nevertheless, full documentation of the approach adopted within the NIS software package–that provided the general basis of the development of ENBIOS–can be used to provide an overview of the file and how it functions (see (Magic Nexus, n.d.)).

In any case, the file does contain certain information that may need to be changed or adjusted when setting up different scenario simulations. Perhaps the most likely of these involves the specification of the life cycle inventory (LCI) data that is to be applied at each of the structural processors. LCI data is provided in the form of .spold files. These files contain detailed inventories of all of the inputs and outputs to the process that applies at each structural processor node. Accordingly, the name of the .spold file that applies at each structural processor needs to be specified in the '@EcoinventFilename' column of the 'BareProcessors top levels' sheet for every instance where 'Structural' is specified in the 'FunctionalOrStructural' column. As these inventories can be derived based on different amounts of energy (e.g., some are supplied in the databases per kWh, while others are supplied per MJ or other units) a factor must be applied to convert the data within the inventories to a common reference unit. In the SENTINEL project, the common unit is assumed to be one EJ and these factors are listed for all structural processors in the '@EcoinventEJ' column.

Other columns may also need to be specified in this sheet, as follows:

- @EcoinventName – String to describe name of process that .spold file relates to. For reference only – not used in calculations
- @Combustion_kgCO2_EJ – The combustion factor for calculating kg of CO2-eq when directly combusting fuels. This column is for fuels where consumption is provided in EJ
- @Combustion_kgCO2_kg – As above but used for fuels where consumption is provided in kg

Data from other sheets may also need to be changed for some simulations. These sheets and their functions are as follows:

- 'ParametersRawMaterials' – Specifies the raw materials to be included in the raw materials output calculations and the three parameters for each of these materials. The value of each parameter is listed in 'Value' column, while the parameter type is specified in the 'Group' column. The three parameters are as follows:
    - 'EUMaterialsConsumption' – The total amount of each material consumed in the EU in the reference year 2016 (Bobba et al., 2020; European Commission, 2020a)
    - 'MaterialsSupplyRisk' – Supply risk factor as given in (European Commission, 2020b)
    - 'MaterialsRecyclabilityRate' – End-of-life recycling input rate (EoL-RIR) as given in (European Commission, 2020b)
- 'LCIAMethods' – Specifies the life cycle impacts assessment (LCIA) methods to be used and several related parameters. Can most likely be left as default listings

3.2 Life cycle assessment data and methods

Two types of LCA-related inputs are required in order to prepare a simulation of ENBIOS. Firstly, the LCI inventory data must be converted from the native .spold format into a NIS-compatible file. Secondly, a list of the LCIA methods must be converted into a NIS-compatible file.

3.2.1 LCI inventory data

Data from the .spold files that define the inventories at each of the structural processor nodes can be converted into a NIS-compatible summary file using the `lci_to_nis` action. This requires the following parameters to be specified:

- `spold_files_folder` – Local path of the folder where all .spold LCI files are located
- `correspondence_path` – Currently not used. Specifies the path of a .csv file in which a mapping from technologies to .spold files and from technologies to the MuSIASEM dendrogram can be defined
- `nis_base_url` – Location of 'Base' workbook file where 'BareProcessors' commands will be scanned to look for mapping information that links structural processors with .spold files. Note that if the 'Accounted' property in the file is set as 'No', .spold filename specified for the specified 'ParentProcessor' will be taken. It is assumed that this will be the URL of a shared online file. However, a local file can also be used, if prefixed by file://
- `nis_structurals_base_path` – Local path where the output NIS file will be generated

Example:

```
enbios lci_to_nis /home/enbios/spold_files/ ""
https://docs.google.com/spreadsheets/d/15NNoP8VjC2j1hktT0A8Y0ljqOoTzgar8l
42E5-IRD90/edit?usp=sharing /home/enbios/lci_to_nis_output.xlsx
```

When the process is completed, the resulting.xlsx file should be moved to the required shared folder (in case of collaborative work). This link should then be copied into the 'ImportCommands LCI Structurals' sheet in the 'Base' workbook file.

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3.2.2 LCIA methods

Similarly, to integrate the selected LCIA method data into ENBIOS, an action is required to convert the raw LCIA method data into a NIS-compatible file. This action is known as `lcia_implementation_to_csv` and requires the following two parameters to be specified:

- `method_file` – The path of the input .xlsx file containing LCIA method information
- `lcia_file` – The path of the output .csv file

Example:

```
enbios    lcia_implementation_to_csv    /home/enbios/lcia_method_in.xlsx
/home/enbios/lcia_method_out.csv
```

The resulting .csv file should contain the following columns:

- 'LCIAMethod' – Identifier of the LCIA method
- 'LCIAIndicator' – Identifier of the LCIA indicator (e.g., 'GWP' for Global Warming Potential)
- 'Interface' – The name of the exchange whose value will be picked from each considered activity (processor) for the weighting
- 'InterfaceUnit' – The unit expected for the 'Interface' value
- 'LCIAHorizon' – When the ReCiPe method is chosen, the 'cultural perspective' employed in the ReCiPe method according to Huijbregts et al. (2017):
  - 'I' – Individualist
  - 'H' – Heirarchist
  - 'E' – Egalitarian
- 'LCIACoefficient' – The weighting factor
- 'Compartment' – Specifies to which environment compartment the weighting applies

As with the LCI file in the previous step, the resulting file should be moved to the required shared folder (in case of collaborative work). This link should then be copied into the 'ImportCommands LCI Structurals' sheet in the 'Base' workbook file. Then, where appropriate, listings from this file should be copied into the 'DatasetDef', 'LCIAMethods' and 'ScalarIndicators' sheets in the 'Base' workbook file.

3.3 System data for individual scenarios

ENBIOS is capable of running simulations of many scenarios which, by their nature, will require different levels of different elements within the energy system to be specified. That is, a simulation for one scenario may contain a certain amount of electricity supplied from wind turbines–and all other sources of energy–while the next will specify different amounts of this energy. As ENBIOS is designed to be able to simulate many different scenarios, a way to input the different distributions or 'energy mixes' into the software is required.

Prior to running a simulation, this data is entered into the 'BareProcessors simulation' sheet of the 'Base' workbook file. For small changes or troubleshooting runs, these changes could be entered directly into the cells of this sheet. However, the software has mainly been developed to analyse energy system data for various scenarios to be provided by other members of the SENTINEL project. As such, a methodology was required to convert the complex sets of data to be provided into simplified sets of compatible data that can be used to define and simulate scenarios in ENBIOS.

The solution adopted has been to provide an action capable of scanning simulation datasets to elaborate a report workbook in which the different elements considered in the simulation are enumerated: regions, scenarios, times, technologies, carriers, measures (interfaces), etc. Here, the action is known as `enbios sentinel_to_nis`. The required parameters for this action are as follows:

- `sentinel_data_package_json_path` – The path to the index .json file containing the simulation results from other SENTINEL simulations. The file will use the so-called 'friendly_data' definitions that follow a common nomenclature for elements of the energy system to be used by all partners within the project
- `nis_file` – The local path where the output report workbook will be generated

Example:

```
enbios                                                     sentinel_to_nis
/home/enbios/case_study_1/sentinel_output/datapackage.json
/home/enbios/case_study_1/sentinel_output/
```

Table 7 Summary of required ENBIOS inputs

Feature	Command(s)	Source	Comment
Processors (MuSIASEM dendrogram)	'BareProcessors top levels'	Manually transcribed from graphical dendrogram	Hierarchical schema of the energy sector
InterfaceTypes (MuSIASEM)	'InterfaceTypes'		Types of biophysical flows between processors
Raw material factors	'Parameters Raw Materials'	Data manually written into workbook	
Scalar indicators	'ScalarIndicators'	Non-LCIA indicators are manually specified from the outcome of analytical process	Indicators attached to each structural processor
Provenance references	'RefProvenance'	Manually	Useful to annotate the sources used in interface values

Feature	Command(s)	Source	Comment
Geographic references	'RefGeographic'	Manually	Useful to annotate location of processors using NUTS codes
LCI database	File location in 'ImportCommands LCI structural. File contains information relating to: 'InterfaceTypes', 'BareProcessors top levels' and 'Interfaces'	Workbook generated by `lci_to_nis`	A database of LCI activities used to provide raw LCI information to individual structural processors
LCIA methods	'DatasetDef', 'LCIAMethods', 'ScalarIndicators'	lcia_method_in.xlsx -> `enbios lcia_implementation_to_csv` -> lcia_method_out.csv	
Energy 'mix' at structural processors	'BareProcessors simulation'	Use results from `sentinel_to_nis`. 'Processor' categories and data from SENTINEL outputs should be aligned to the structural processors in 'BareProcessors top levels' using the 'Parent Processor' column	Provides integration between SENTINEL simulation results and MuSIASEM and LCA functions in ENVIRO

As with the LCA data and methods in the previous sections, listings from the resulting file should be copied into the appropriate locations in the 'BareProcessors simulation' sheet within the 'Base' workbook file. Each output from the SENTINEL database must be matched with the appropriate corresponding structural processor from the 'BareProcessors top levels' sheet. This is done by defining the 'link' in the 'ParentProcessor' column of the 'BareProcessors simulation' sheet.

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4 Execution of simulations

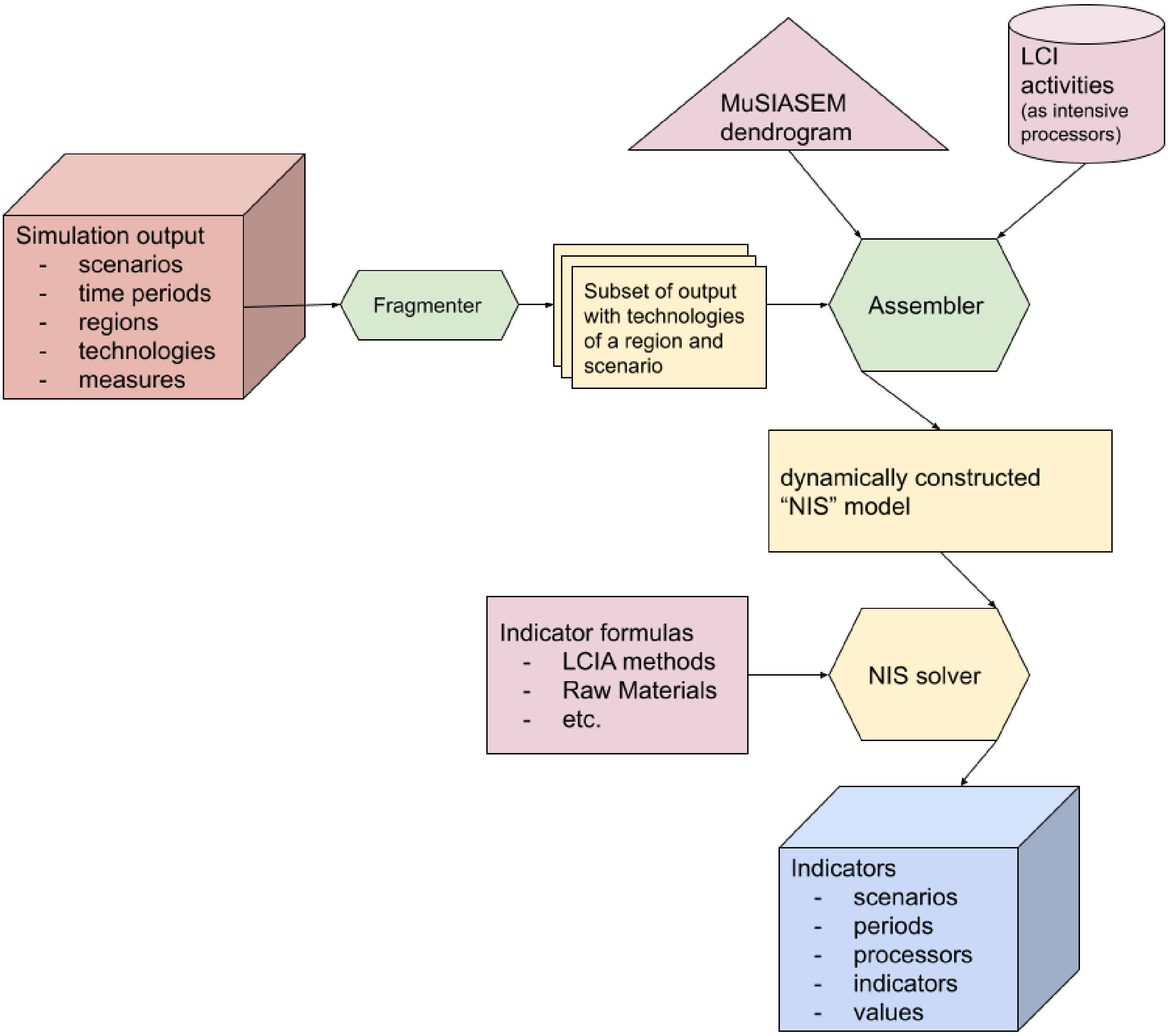
Once the inputs detailed in section 0 have been prepared, the final action can be executed. The steps carried out by this action are as follows:

- Read the 'Base' model from the 'Base' workbook file. The model provides:
    - Database of reference LCI processors
    - Information on how to associate technology names (from simulation) with LCI processor information
    - Information on how to associate technology names with MuSIASEM processors
    - How to calculate indicators
    - How to elaborate intermediate outputs
- Split the simulation into separately processable pieces. Fragmentation is performed by 'Scenario' and 'Region'. Time/year could be performed in future, but is as yet untested
- For each simulation fragment, generate a fragment-model (NIS file):
    - For each technology:
        - Gather interfaces coming from the simulation and create a processor with those interfaces
        - Find the main output of the technology
        - Find an LCI processor for each technology and copy the interfaces, making them relative to the simulation output instead of the LCI reference output (assume they are the same)
        - Find a MuSIASEM parent for the technology and assign it to that parent
    - Generate a NIS model file
    - Submit this dynamically generated NIS model, and calculate LCIA and other indicators
    - Collect and accumulate results

Figure A presents a simplified flowchart for this procedure. The 'Simulation output' box represents the data package of outputs from other SENTINEL models that act as the changing energy system inputs to be considered in ENVIRO. This data then enters the 'fragmenter' process, to produce accountable fragments in parallel. Each fragment then enters an 'assembler' process–considered to be the core of ENVIRO–which generates a model incorporating and integrating information from the MuSIASEM dendrogram and information extracted from the LCI files. The assembled model is then injected into a process called 'NIS solver' which propagates available quantitative information and calculates indicators arranging them in the output dataset.

In Figure A , the salmon-coloured pieces of information come from the 'Base' workbook. The green, hexagonal processes are undertaken within the ENBIOS and NEXINFOSYS (NIS) packages. The blue output dataset at the bottom of the figure has similar dimensions to those from the SENTINEL input data package adding indicators instead of measures to technologies and incorporating the processors from the MuSIASEM dendrogram.

Figure A 1 Conceptual flowchart for ENBIOS



ENBIOS simulations are executed as follows:

```
enbios enviro /home/enbios/enviro_run_1.yaml --just_one_fragment=True
```

The .yaml configuration file, technically known as 'cfg_file_path', contains the following variables:

- 'nis_file_location' – The URL of the 'Base' workbook file

- 'correspondence_files_path' – Currently not used. Could be used to define the path of a .csv file in which a mapping from technologies to .spold files and from technologies to the MuSIASEM dendrogram could be specified
- 'simulation_type' – States the file format of the simulation input. For now, should always be 'sentinel'
- 'simulation_files_path' – Path to the reference file or folder needed by the specific simulation output format. In the case of 'sentinel', it should be the path of the index .json file used by the 'friendly_data' package to drive the reading of the simulation results
- 'output_directory' – Path of the local directory where all outputs of the execution will be placed

An example .yaml configuration file is given below:

```
nis_file_location:
"https://docs.google.com/spreadsheets/d/15NNoP8VjC2jlhktT0A8Y0ljqOoTzgar8
l42E5-IRD90/edit?usp=sharing"

correspondence_files_path: ""

simulation_type: sentinel

simulation_files_path:
"/home/enbios/case_study_1/sentinel_output/datapackage.json "

output_directory: "/home/enbios/case_study_1/enviro_output/"
```

A number of execution driving flags can also be placed after the .yaml filename, as follows:

- `just_one_fragment` – If 'True', only the first fragment of the split simulation data will be processed. This reduces simulation time and is useful for troubleshooting. 'False' by default
- `generate_nis_base_url` – Because the 'Base' framework model can be quite large, it is possible to have specification issues. If this parameter is set to 'True', a workbook in NIS format is generated returning information on how NIS interprets "Base". 'False' by default
- `generate_nis_fragment_file` – If 'True', for each fragment the dynamically generated NIS file is written to the output directory. 'False' by default
- `generate_indicators` – If 'True', a separate indicators.csv file is written for each of the fragments (the aggregate indicators .csv file is always generated). 'False' by default
- `max_lci_interfaces` – If >0, when LCI interfaces are merged into simulation processors, the number of interfaces cannot exceed this parameter. This is useful when checking the system prior to a full execution. By default, this is set to 0, meaning 'all interfaces' are activated

5 Results

The main output of the process is an 'indicators.csv' file which details the indicator results for each defined processor. The file contains the following columns:

- 'Scenario' – To which scenario, coincident with SENTINEL scenario codes, do the indicator values apply
- 'Period' – As above, but relating to time period
- 'Scope' – Scope of the indicator. Can be 'Local' (domestic), 'External' (imports/exports) or 'Total'. Currently only 'Local makes sense'; other rows can be filtered out
- 'Processor' – The processors to which the indicator applies
- 'Indicator' – Name of the indicator
- 'Value' – Value of the indicator

Note that there is currently no 'Region' column, although this could be added in the future, if required.

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