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PROPOSAL OF A MODELLING FRAMEWORK FOR PROSPECTIVE HYBRID LIFE  
CYCLE ASSESSMENT AND APPLICATION TO A NOVEL BIOREFINERY  
SYSTEM

**Presentata da:** Roberto Porcelli

**Coordinatore Dottorato**

Michele Cicoli

**Supervisore**

Andrea Contin

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## List of abbreviations

ALCA	Attributional Life Cycle Assessment
AP	Acidification Potential
BAU	Business As Usual
CLCA	Consequential Life Cycle Assessment
EEIOA	Environmentally Extended Input-Output Analysis
EP	Eutrophication Potential
EU	European Union
GWP	Global Warming Potential
HDO	Hydro De-Oxygenation
HTP	Human Toxicity Potential
IEA	International Energy Agency
IO	Input-Output
IOA	Input-Output Analysis
IOT	Input-Output Table
ILCD	International Reference Life Cycle Data System
JRC	Joint Research Centre (of the European Commission)
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MFA	Material Flow Analysis
POCP	Photochemical Ozone Creation Potential
PSA	Pressure Swing Adsorption
RED	Renewable Energy Directive
RoW	Rest of the World
SETAC	Society of Environmental Toxicology and Chemistry
TBL	Triple Bottom Line
TCR	Thermo-catalytic Reforming
TSF	To-Syn-Fuel (H2020 Project)
UNEP	United Nations Environment Programme

## English Abstract

Measuring progress towards environmental sustainability requires appropriate frameworks and tools. Product-related sustainability tools focus on flows in connection with production and consumption of goods and services. In this category, life cycle assessment (LCA) represents the most established and well-developed tool, relying on an internationally standardised methodology (ISO 14040 and ISO 14044) for the quantification of product's impacts through all phases of its life cycle. However, despite the standardisation has contributed to its broad acceptance and wide use, several limitations have been pointed out over the past years; as a consequence, LCA is still undergoing an intense research effort. More specifically, conventional LCA, due to its static and linear framework, is poorly suited for measuring the broader environmental consequences of an action which unfolds over a large period of time, during which conditions may change revealing different effects from those on the short-term. Indeed, the environmental performance associated to a product system can be quite sensitive to its context and other systems' response in the economy; furthermore, in a rapidly changing world this context can vary considerably over time.

The general objective of this research is to develop an advanced LCA framework to be used as a supporting tool for decision-making. The case study for the application of the proposed framework is the novel biorefinery system currently investigated in European H2020 project To-Syn-Fuel, acronym for "The demonstration of waste biomass to Synthetic Fuels and Green Hydrogen". The ambition of this project is to demonstrate the technical and economic viability, as well as the environmental and social sustainability, of the integrated approach which combines Thermo-Catalytic Reforming (TCR) technology, a thermochemical process of biomass conversion, to Pressure Swing Adsorption (PSA) process and Hydro-deoxygenation (HDO) processes. The integrated TCR-PSA-HDO process is expected to enable the production of a fully equivalent gasoline and diesel substitute, and green hydrogen for use in transport. Moreover, excess electricity produced by the energy conversion of syngas and biochar can be sold to the grid, and phosphorus can be recovered from residual ashes of biochar, resulting in additional products provided by the integrated biorefinery system.

The goal of the present environmental assessment is to measure the environmental consequences of the decision to implement the TCR-PSA-HDO technology in Europe (compared with business as usual), according to the targets for future market deployment envisaged by the To-Syn-Fuel project.

The proposed framework combines the use of process-based data, input-output data and dynamic scenarios, which can be included in one single tool to go beyond the modelling limitations and

simplified assumptions of a conventional LCA. Practically, a dynamic hybrid input-output table is built, reflecting the gradual implementation of the technology over time and the evolution of future energy scenarios. Global impacts, calculated through input-output environmental extensions, are ultimately compared with the ones associated with a “business as usual” reference scenario, represented by the global system operating without the decision to include the novel technology. The results show how the consideration of both dynamic scenarios and extended system boundaries in one single modelling tool can reveal important contributions in the comparative assessment of impacts. In conclusion, this work demonstrates the importance of measuring environmental sustainability not as intrinsic property of products, but as a feature strictly dependent on the context and its dynamics.

## **Abstract in italiano**

Misurare i progressi verso la sostenibilità ambientale richiede strutture e strumenti adeguati. Gli strumenti di sostenibilità relativi ai prodotti si focalizzano sui flussi connessi alla produzione e al consumo di beni e servizi. In questa categoria, l'analisi del ciclo di vita (LCA) rappresenta lo strumento più consolidato e ben sviluppato, basandosi su una metodologia standardizzata a livello internazionale (ISO 14040 e ISO 14044) per la quantificazione degli impatti del prodotto in tutte le fasi del suo ciclo di vita. Tuttavia, nonostante la standardizzazione abbia contribuito alla sua ampia accettazione e al suo diffuso utilizzo, negli ultimi anni sono state evidenziate diverse limitazioni e la LCA è ancora oggetto di un intenso sforzo di ricerca. Più specificamente, la LCA convenzionale, a causa della sua struttura statica e lineare, è poco adatta per misurare le più ampie conseguenze ambientali di un'azione che si svolge su un lungo periodo di tempo, durante il quale le condizioni al contorno possono mutare rivelando effetti diversi da quelli a breve termine. In effetti, le prestazioni ambientali associate a un sistema prodotto possono essere abbastanza sensibili al suo contesto e alla risposta di altri sistemi nell'economia; inoltre, in un mondo in rapida evoluzione questo contesto può variare notevolmente nel tempo.

L'obiettivo generale di questa ricerca è sviluppare un framework di LCA avanzata da utilizzare come strumento di supporto per il processo decisionale. Il caso studio per l'applicazione del framework proposto è l'innovativo sistema di bioraffineria attualmente analizzato nel progetto europeo H2020 To-Syn-Fuel, acronimo di "The demonstration of waste biomass to Synthetic Fuels and Green Hydrogen". L'ambizione di questo progetto è dimostrare la fattibilità tecnica ed economica, nonché la sostenibilità ambientale e sociale, dell'approccio integrato che combina la tecnologia di reforming termocatalitico (TCR), ossia un processo termochimico di conversione della biomassa, a un processo di Pressure Swing Adsorption (PSA) e un processo di idro-deossigenazione (HDO). Il processo combinato TCR-PSA-HDO consentirebbe la produzione di un sostituto del tutto equivalente a benzina e diesel sostitutivi, oltre a idrogeno "green", da utilizzare nei trasporti. Inoltre, l'elettricità in eccesso prodotta dalla conversione energetica di syngas e biochar può essere venduta alla rete e il fosforo può essere recuperato dalle ceneri residue di biochar, così ottenendo prodotti aggiuntivi forniti dal sistema di bioraffineria integrato.

Lo scopo della valutazione ambientale è misurare le conseguenze ambientali della decisione di implementare la tecnologia TCR-PSA-HDO in Europa (rispetto al "business as usual"), secondo gli obiettivi per la futura commercializzazione previsti dal progetto To-Syn-Fuel.



Il framework proposto combina l'uso di dati basati sui processi, dati di input-output e scenari dinamici, che possono essere inclusi in un unico strumento per andare al di là dei limiti di modellazione e le assunzioni semplificate di una LCA convenzionale. Operativamente, viene costruita una tabella dinamica ibrida input-output, che riflette la graduale implementazione della tecnologia nel tempo e l'evoluzione dei futuri scenari energetici. Gli impatti globali, calcolati attraverso estensioni ambientali input-output, vengono infine confrontati con quelli associati a uno scenario di riferimento “business as usual”, rappresentato dal sistema globale che opera senza la decisione di includere la nuova tecnologia. I risultati mostrano come la considerazione di scenari dinamici e confini estesi del sistema in un unico strumento di modellazione possa rivelare importanti contributi nella valutazione comparativa degli impatti. In conclusione, questo lavoro dimostra l'importanza di misurare la sostenibilità ambientale non come proprietà intrinseca dei prodotti, bensì come una caratteristica strettamente dipendente dal contesto e dalle sue dinamiche.



# 1 Introduction: environmental sustainability and life cycle assessment

## 1.1 Environmental sustainability

The growing concern on global environmental problems has brought a great focus on the concept of sustainability. Rooted back in 1987 to the United Nations' Brundtland Commission Report "Our Common Future" [1], nowadays sustainability is largely accepted as a paradigm and, extensively, a desirable condition to be achieved pursuing *sustainable development*, defined in the above mentioned report as "development that meets the needs of the present without compromising the ability of future generations to meet their own needs". Although it started as an ecologically based concept, it subsequently evolved forward a more comprehensive idea, being framed into fundamentally three dimensions: environmental, social and economic. The three pillars of sustainability are often indicated as Triple Bottom Line (TBL), when referring to a business perspective which addresses not merely profit maximisation but also people and planet issues, such as social equity and environmental protection [2]. However, in a global perspective, the economic aspect of sustainability results to overpower the environmental and social ones. Nonetheless, the new green economic vision considers the environment as a comprehensive system, where the society is nestled inside, and the economy in turn is seen as a part of the society [3]. This vision implies that environmental sustainability is a prerequisite, a necessary condition for any social and economic sustainability.

At the same time, we witness a conflict between the wellness of the environment, on the one hand, and industrial and technological development, on the other. Human activities have undeniable harmful effects on the environment, and this growing awareness is pushing towards the adoption of greener technological solutions, able to minimise the pressure on the environment. This progress towards environmental sustainability necessarily involves radical changes. One of the main challenges is related to the strong and still increasing hunger for energy in the world, which has been

mainly being fed by fossil fuels, the real engine of industrial revolution in the last two centuries. This strong dependence on a strictly non-renewable (therefore non sustainable) source of energy has always been recognised as a serious issue, but the dominant concern in the last years has become the related impact in terms of climate change, of which anthropogenic emissions of carbon dioxide from fossil fuels combustion are the main responsible [4].

However, besides climate change the planet faces many environmental issues, that can be resumed with reference to *planetary boundaries*, a recently proposed framework ascertaining the existence of global limits for the biosphere, to not overcome in order to guarantee human prosperity [5]. Consequently, as any human activity can do harm to the environment in many different ways, it is requested an analysis which is able to evaluate the environmental sustainability with reference to many different potential impacts, avoiding the shifting from one impact to another. In addition, any activity should be analysed considering the systems involved and their complex structure. In this effort is crucial the adoption of systems thinking, defined as “the ability to see the parts of bigger mechanisms and recognising patterns and interrelationships” [6]. The assessment of the environmental sustainability requires appropriate and commonly shared metrics by the scientific community, setting goals to be reached to let our society remain within a safe operating space.

## 1.2 Sustainability assessment tools

Sustainability science evolved in the attempt to provide efficient and reliable tools to reach the goal of transition to a more sustainable future. As put by *Devuyst et al. (2001)* [7], sustainability assessment can be defined as “a tool that can help decision-makers and policy-makers decide which actions they should or should not take in an attempt to make society more sustainable”. Practically, a multitude of diverse tools and methods have been developed and proposed. Their variety depends on the type of application, scope, scale and level of detail for the system to be analysed, but also on the scientific background of their developers. At the same time, the tools share the same founding principles: integrated analysis of systems, recall of basic physical principles, use of indexes and indicators to present the results. A non-comprehensive list [8] may include:

- Material flow analysis (MFA)
- Input-output analysis (IOA)
- Environmental risk analysis (ERA)

- Environmental impact assessment (EIA)
- Life cycle assessment (LCA)
- Ecological footprint

Some of these methods share a similar methodological background. For instance, MFA, IOA and LCA have in common the attempt to model the complexity of production and consumption systems in order to trace source impacts to a functional demand [9]. The existing overlap among different fields can be exploited identifying possible synergies [10].

## 1.3 Life Cycle Assessment

Product-related tools focus on flows in connection with production and consumption of goods and services. The most established and well-developed tool in this category is life cycle assessment (LCA) [11]. It is an internationally standardised methodology which allows for the quantification of environmental impacts associated to any good or service (both referred as “product”) considering all phases of its life cycle, which can include raw material acquisition, production, transportation, use and products’ end-of-life [12].

In the European context, LCA has been recognised as the most appropriate framework for assessing the potential environmental impacts of products [13]. Starting from its origins as a micro-level company based tool, it has evolved expanding its range to larger scale decision contexts, for example to help design national energy solutions [14]. Therefore, more recently it has been also indicated by European Commission as a pertinent tool to support public policy making [15] [16].

The ISO 14040:2006 standard [12] describes the principles and framework for LCA, including four main phases to be followed: (1) goal and scope definition, (2) life cycle inventory (LCI) analysis, (3) life cycle impact assessment (LCIA) and (4) interpretation. In particular, LCI involves the collection and analysis of environmental interventions data, i.e. inputs from the environment (resources) and outputs to the environment (emissions), which are associated with a product throughout its life cycle; LCIA subsequently associates the inventoried environmental interventions to potential environmental impacts, e.g. global warming, resource depletion, acidification, expressing them through a set of indicators. ISO 14044:2006 standard [17] completes ISO14040 specifying requirements and providing guidelines.

However, despite the standardisation has contributed to its broad acceptance and wide use, LCA is still undergoing an intense effort of research and development. The life cycle thinking appears to be

a fundamental principle on which to rely on, in order to evaluate a product through a holistic view, since it allows to avoid burden shifting from one process to another along a supply chain, and from one environmental problem to another, accounting for different type of impacts. However, other requirements can be important as well. The analysis could allow considering future boundary conditions like changes in technological and economic surroundings. System wide changes could be considered beyond the physical product supply chain. A change-oriented than a descriptive analysis in some situations could more appropriate.

## **1.4 Limitations of LCA**

Many LCA practitioners and researchers argue that the ISO14040-44 standards do not provide enough guidance for many practical aspects of the LCA procedure [18] [19], leaving too much room for subjective interpretation and remaining vague on key methodological points [20]. This criticality has been partially settled through the issuance of additional guidelines. The most important contribution on this side was brought by the Institute for Environment and Sustainability in the European Commission Joint Research Centre (JRC), which developed the International Reference Life Cycle Data System (ILCD) Handbook [21], a series of technical guidance documents to the ISO 14040-44 standards. However, also this guide is not exempt from criticism [22] and many issues remain open. A systematic review of the limitations of LCA has been done, in particular, through the European project CALCAS [23], which aimed at identifying research lines on life cycle analysis approaches in supporting the sustainability decision making process.

In the following, the main methodological issues identified in the CALCAS project are resumed and updated with new and additional contributions by the scientific literature.

### **1.4.1 Linear modelling**

Both the inventory analysis and impact assessment phases in LCA are based on linear modelling [24]. In the first case, it means that all processes included in the system are supposed to shrink or expand with fixed proportions among its inputs and outputs. In the second case, it means that ecological processes respond in a linear manner to environmental interventions and thresholds of interventions are disregarded, which implies a linear relationship between the increase in an environmental intervention and the consequent increase in the associated impact.

The linear assumption in inventory models collides with real world technological processes, which usually do not have standard “recipes” but are subjected to economies of scale or can face supply-side constraints. However, including non-linear production functions in the process network for building the LCI would likely result in an unmanageable model, considering the high number of processes normally involved in a product system. The focus can be then shifted on data collection: if average data are used for a certain process, it means that the “recipe” will reflect the average of existing conditions for that process; however, in some situation marginal data are more appropriate, since in this case the “recipe” will reflect the effect of a change in production. A typical example is agricultural production: assessing the impact of the actual production of a certain agricultural product would involve the understanding of existing conditions, therefore the average data can be a good option. On the contrary, if the objective is to assess the impact related to an increase in production to meet additional demand of that product, e.g. used for producing biofuels, one should seek for marginal data for the process of agricultural production. Indeed, farmers would meet additional demand in different ways, for example applying more fertilisers to increase crop yields, not necessarily increasing the use of pesticides and water in the same proportions, or more land will be converted to produce that crop in place of other previous uses of that land, and therefore land use changes should be investigated. This not necessary implies changing the basic linear structure of the LCA model, but it would mean seeking for different information and data to feed the model [25].

## 1.4.2 System boundaries definition

The choice of the system boundary pertains to the first phase of LCA, Goal & Scope definition. In the ISO14040, system boundary is defined as a “set of criteria specifying which unit processes are part of a product system”. Also, LCI result is defined as the “outcome of a life cycle inventory analysis that catalogues the flows crossing the system boundary and provides the starting point for life cycle impact assessment” [12]. In this regard, it is important to clarify that, as noted by *Guinée et al. (2002)* [26], three major types of system boundaries in the LCI exists:

- between the technosphere and the environment;
- between the technological system under study and the rest of the technosphere;
- between significant and insignificant processes.

The first type refers simply to the need to trace flows (called “intermediate flows”) throughout the life cycle, until the system analysed only exchanges flows with the environment, called “elementary

flows” in the ISO standards. The identification of this type of boundary is obvious in many cases, so this is generally not regarded as a big issue, although in some cases it is not totally straightforward (e.g. waste and landfill emissions) [27].

The second type pertains to the problem of understanding which part of the technosphere is involved in the function under study, which has always been a major issue in LCA, in particular with regard to multifunctional processes. There are principally two ways of handling multifunctionality [27]: allocation and substitution (or system expansion, see 2.3.1). The first method consists in assigning to each function of the process a fraction of its impacts, with an allocation rule which can be based on physical, economic or other properties reflecting the respective value attributed to each function. For example, when an industrial process has two products as outputs, both with an economic value, its impacts can be assigned to each product on the basis of their selling price. Instead, substitution consists in including affected parts of other life cycles in the technological system under study and subtract their environmental impacts. For example, if the function of the system is waste management through incineration, which provides the additional function of producing electricity, the system will include the avoided production of electricity through other technologies, and account for the corresponding avoided impacts.

The third type of system boundary is related to the practical need of introducing a cut-off criterion to exclude processes which are presumably not very significant for the analysis. This is necessary because the global technological system is composed of activities highly interrelated, and the ideal situation in which the product system only exchanges flows with the environment, as prescribed by ISO standards, can never be reached in practice. In the ISO14040 it can be read: “Ideally, the product system should be modelled in such a manner that inputs and outputs at its boundary are elementary flows. However, resources need not be expended on the quantification of such inputs and outputs that will not significantly change the overall conclusions of the study” [12]. The fallacy of this reasoning stands in the fact that there is not a scientific way to know in advance which parts of the system can be excluded being not significant for the results. Thus, applying a cut-off rule, e.g. by mass or energy, is a necessary practice but it remains difficult to scientifically justify. The omission of contributions left outside the boundary introduces in the analysis a systematic error, defined truncation error, which may result in a significant underestimation in the LCI, sometimes referred to as “incomplete system boundaries” [28].



### 1.4.3 Time dimension

Classical LCA modelling relies on steady-state conditions: time dimension is not explicitly considered, and time variability is not foreseen by the model. As a result, LCIs do not include any information on the time of occurrence of emissions and resource uptake, and consequently the impacts which can be calculated represent the sum of impacts over the time horizon considered. According to ISO14040 [12] “environmental data are integrated over space and time”; moreover, “the lack of spatial and temporal dimensions in the LCI results introduces uncertainty in the LCIA results. The uncertainty varies with the spatial and temporal characteristics of each impact category”. As can be seen, the lack of time dimension is acknowledged as a method’s limitation.

Consideration of time dimension can involve many different aspects of a life cycle analysis and can be addressed in many ways. Indeed, it can range from the consideration of different prospective scenarios in LCI over the time horizon of the assessment [29] to the temporal differentiation for processes along a supply chain, unveiling the distribution over time of environmental interventions related to a product life cycle [30]. The consideration of a time-dependent LCI can be a premise for consideration of time dimension in the LCIA phase, such as the use of dynamic characterisation factors.

*Lueddeckens et al. (2020)* [31] performed a systematic review of temporal issues in LCA. They recognised six types of temporal issues, namely time horizon, discounting, temporal resolution of the inventory, time-dependent characterisation, dynamic weighting, and time-dependent normalisation. They concluded saying that not considering these issues “is a simplification that in some cases can have decisive influence on the outcome of LCA, potentially leading to wrong decisions”.

However, attempts to develop a dynamic LCA have been battling with methodological and practical difficulties, mainly as a result of the fact that the available software tools are generally based on static relations and are not supported by databases that could be representative of future situations. Even when a model is found to be theoretically valid, there remains the challenge linked to the retrieval and management of temporal information for the system description and modelling [32].

# 1.5 Advanced LCA approaches

## 1.5.1 Consequential LCA

The ISO14040 [12] recognises the existence of two possible approaches to LCA, with different purposes:

- *one which assigns elementary flows and potential environmental impacts to a specific product system typically as an account of the history of the product, and*
- *one which studies the environmental consequences of possible (future) changes between alternative product systems.*

Although this clarification is relegated to the margin of the document and liquidated in a nutshell, this is a major topic in the LCA community, having generated a lot of debates and discussion, but which remains still an unresolved matter.

The first approach responds to a more traditional way to consider life cycle assessment. The second approach corresponds to a new perspective which emerged subsequently. The two approaches have been defined, respectively, “attributional” and “consequential”. The terminology was coined in 2001 [33], but the origin of this duality can be found in the early nineties, when a fervent debate emerged on the limitations of LCA in capturing market-driven aspects, mainly due to its narrow focus on physical relationships [34] [35]. A brief history of the concept and the associated long-running debate is provided in Fig. 1.

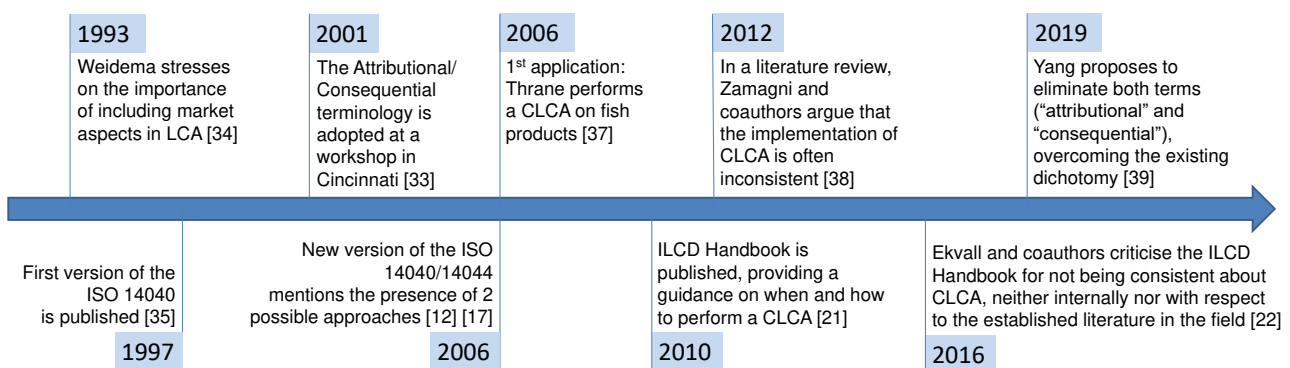


Fig. 1 – Key milestones in the debate upon the consequential concept

The first attempt to conceptualise consequential LCA (CLCA) can be attributed to Bo Weidema [34] [40] [41], who attempted to illustrate the conceptual difference between attributional LCA (ALCA) and CLCA in a simple but meaningful figure:

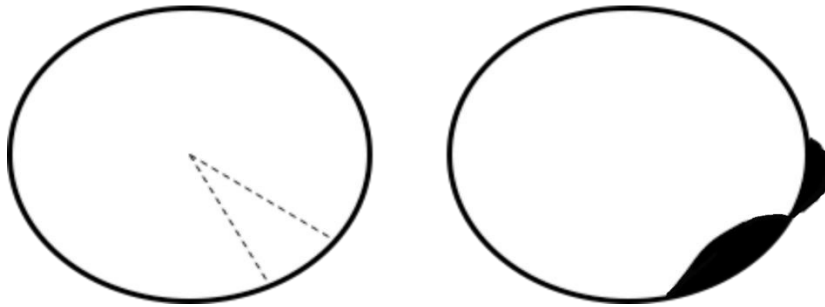


Fig. 2 - *The conceptual difference between attributional and consequential LCA* [40]

The circles in Fig. 2 represent the total global environmental exchanges. In the left circle, attributional LCA seeks to cut out the piece with dotted lines that belongs to a specific human activity. In the right circle, consequential LCA seeks to capture the change in environmental exchanges that occur as a consequence of adding or removing a specific human activity [40].

Different “official” definitions for the two concepts can be found. The most relevant are those provided by the JRC and the UNEP/SETAC in their respective guidelines.

The ILCD Handbook [21] by the JRC provides a guide to the choice and application of the two modelling approaches, defined as follows:

- *The attributional life cycle model depicts its actual or forecasted specific or average supply-chain plus its use and end-of-life value chain. The existing or forecasted system is embedded into a static technosphere.*
- *The consequential life cycle model depicts the generic supply-chain as it is theoretically expected in consequence of the analysed decision. The system interacts with the markets and those changes are depicted that an additional demand for the analysed system is expected to have in a dynamic technosphere that is reacting to this additional demand.*

The UNEP/SETAC guidelines for LCA practice report the following definitions in its glossary:

- *Attributional approach: System modelling approach in which inputs and outputs are attributed to the functional unit of a product system by linking and/or partitioning the unit processes of the system according to a normative rule*

- *Consequential approach: System modelling approach in which activities in a product system are linked so that activities are included in the product system to the extent that they are expected to change as a consequence of a change in demand for the functional unit.*

Indeed, the interpretation of the consequential concept is not unique among the LCA scholars and the applications of CLCA still include a vast range of methods [38]. Probably, the absence of a single standard definition does not help in this sense. The lack of agreement on the concept in the scientific community is manifest when trying to understand the relationship between ALCA and CLCA, based on the authors' statements. In Fig. 3 there is a visual representation of this relationship which can be deduced from various authors.

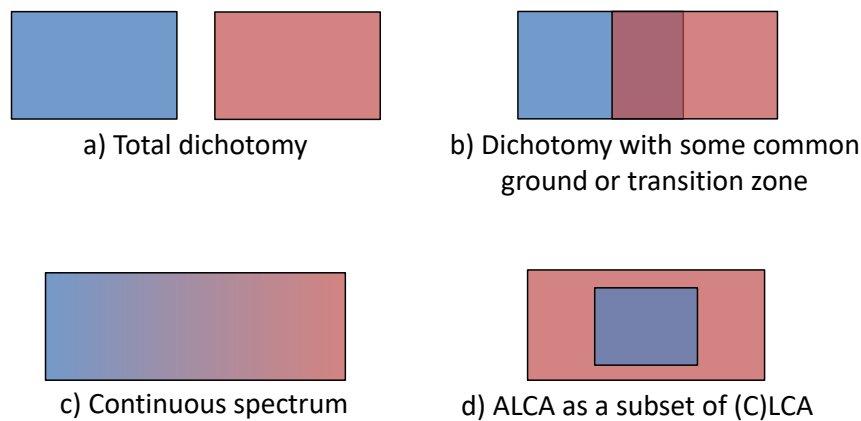


Fig. 3 – *Different views on the conceptual relationship between attributional (in blue) and consequential (in pink) LCA*

The set of studies that would fall under the attributional approach is represented in blue, while the set of studies that would fall under the consequential approach is represented in pink. Many authors, including most of the existing guidelines, refer to the two approaches as if a sharp line could be traced between them, therefore any valid study should fall under one set or the other, according to their view [42] [43]. In particular, the ILCD Handbook [21] explicitly advises to refrain from combining the two approaches. Other authors still consider the existence of two separated sets, but admit the presence of a possible transition zone, so that some studies can be considered a hybrid of the two approaches [38]. Another widespread school of thought regards to the approaches as the two ends of a continuous spectrum, in which usually a full consequential study is never achieved [44] [45]. Finally, *Yang (2019)* [39] argues that LCA is consequential by nature, following the general principle of consequentialism, therefore the term “consequential” is pleonastic and ALCA should be just considered as a particular type of (C)LCA.

As a consequence, also the practical application of the concept tends to follow many different routes. Surprisingly, the nature of CLCA modelling, in terms of analysing principles and analytical techniques used, is a topic only recently discussed in the literature [38].

*Weidema et al. (2009)* [43] clarify that “consequential models are steady-state, linear, homogeneous models, with each unit process fixed at a specific point in time”, although “external dynamic models may be applied to generate input data”. Hence, it can be deduced that ALCA and CLCA share the same modelling principles. However, the identification of unit processes to be included in the system follows different criteria in the two approaches. In the case of ALCA, the processes are included following a descriptive logic, which aims at depicting the reality of the analysed system’s processes and life cycle stages. In contrast, in CLCA the processes included are those that are assumed to be operated as reaction to a change, namely a decision, since it aims at identifying the consequences of a decision in the foreground system on other processes and systems of the economy [21]. The decision may refer to the choice to buy or produce a particular product, the change in a certain production process, or even a policy strategy. Therefore, it can be deduced that ALCA, describing an *actual* supply-chain with a focus on physical relationships, just requires the collection of *actual* (specific or average) data, whereas CLCA, modelling a *hypothetic* supply-chain along market-mechanisms, needs in support economic and dynamic models.

*Palazzo et al. (2020)* [46] refer to “structural models for CLCA”, intending models that specify input parameters and equations that govern the hypothesized cause-effect relationships in the system; the same authors identify in the literature mainly 4 types of these models: (a) economic equilibrium models, (b) systems dynamics models, (c) technology choice models, and (d) agent-based models.

*Yang & Heijungs (2017)* [47] acknowledge this trend in incorporating increasingly sophisticated models in CLCA studies, warning that more mathematical sophistication may not necessarily improve the accuracy, if the models are still based on highly restrictive assumptions. They conclude with two recommendations: (1) not relying on a single class of models, but using the collective estimates of different models, given their different strengths and limitations; (2) focusing more on relaxing some of the restrictive assumptions to improve a model’s predictive capability (which not necessarily implies a mathematical sophistication), e.g. they suggest the use of scenarios instead of simple linear extrapolation when using linear models that assess the consequences of a decision.

Beside the aforementioned inconsistencies, there is a certain agreement on the fact that CLCA should be used for decision-support, especially for meso- and macro-scale decisions. Indeed, the goal of ALCA is considered descriptive of an existing situation and should be used mainly for reporting purposes, while the goal of CLCA is capturing the consequences of changes [48]. Nevertheless, some

authors still argue that CLCA is a superior approach, although introducing more uncertainty [42], and has suggested that it should be used even when dealing with small decisions [49].

From a practical perspective, the main agreement is on two points: (1) the choice of system expansion (or substitution) in order to handle multifunctionality is a necessary condition for performing CLCA, and (2) marginal data shall be used in place of average data [38].

About the first point, it should be noticed that system expansion is widely used also in LCAs of the attributional type, and there are different opinions on the appropriateness of this modelling choice for ALCA. For instance, *Weidema (2003)* [40] argues that “attributional LCA does not involve changes, which is a necessary condition for applying the system expansion procedure”. However, *Zamagni et al. (2012)* [38] point out that use of system expansion is not sufficient to label a study as consequential, although some cases can be found in the literature. *Majeau-Bettez et al. (2018)* [50] thoroughly analyse the problem of coproduction and conclude that “the prevalent dichotomy between partition and ‘system expansion’ is overly limiting and suboptimal for answering attributional and consequential life cycle questions”.

About the second point, it can be said that the inclusion of marginal processes in place of average processes is not limited to a choice of data: various order of consequences can be taken into account, which can go quite beyond the ideal supply chain structure. The ILCD Handbook makes a distinction between primary and secondary consequences. The first type regards both processes “that are operated as direct market consequence of the decision to meet the additional demand of a product” and processes “that supersede/complement co-functions of multifunctional processes that are within the system boundary” (i.e. handling multifunctionality with substitution). Secondary consequences include many types of market mechanisms, such as price effects, which result in increased or decreased demand for competing functions or not required co-functions: this means that effects on other product systems affected through market relationships are included, expanding considerably the system boundaries of the analysis, with a potentially endless chain of consequences that can be analysed. Some studies underline that these secondary effects can go far beyond the direct effects on the main product system along the supply-chain; for example, *Sandén & Karlström (2007)* [51] argue that, when assessing investments on emerging technologies, marginal contributions to radical system changes can be expected and should be included in the analysis, as well as marginal changes in the current system. When secondary effects counteract the primary consequences and partially or completely compensate them, they are regarded as “rebound effects”, at least accordingly to the ILCD Handbook definition: as a matter of fact, while many attempts to address the issue of rebound effects can be found in the CLCA literature, inconsistencies on the definition and classification of the concept

are present among studies [52]. Sometimes the term assumes also more specific meanings: for instance, in the field of biofuels, rebound effect is defined as “the effect that an increased use of biofuels reduces oil demand, which in turn results in a decrease of the price of oil. This oil price decrease leads to higher demand for oil, which causes oil consumption to decrease less than the increase in biofuel use (on energy content basis)” [53]. This phenomenon is also referred to as Indirect Fuel Use Change (IFUC) [54] or Indirect Energy Use Change (IEUC) [55]. While addressing also these types of indirect effects is certainly praiseworthy, this is naively applied in a context of LCA analysis, without considering that, by doing so, the study would depart from the conventional one-to-one perfect substitution ratio; in fact, even the existing guidance on CLCA adheres to the principle of functional equivalence between product systems to apply substitution and ensure comparison on a like-for-like basis [56]. Instead, it should be considered that departing from the assumption of perfect displacement has important implications for the foundations of the methodology. Expanding the boundaries to include processes affected by all kind of consequences, including changes in consumer behaviour or changes in the level of general consumption by consumers due to changes in price, can bring to the comparison of situations serving different functions, consequently it might be difficult to guarantee the functional equivalence between the systems compared [38].

In conclusion, different views persist on the topic and there is no agreement on how to perform properly a consequential LCA. However, many insights emerged from the prolific discussion on the issue, suggesting that the conventional framework based on the attributional approach is too limited in several aspects.

## 1.5.2 Hybrid LCA

The problem of incomplete system boundaries can be addressed mainly in two ways:

- improving the basis for cut-off criteria;
- reducing or eliminating the need for cut-off.

The use of input-output tables is regarded as the most significant of the second type of approach [18]. Indeed, an input-output table is an aggregated model of all activities in the economy, therefore it has the potential to eliminate the need for cut-off.

The idea of modelling all sectors of an economy through a table of inputs and outputs is not new: it was introduced by Wassily Leontief in 1928 [57] [58], and in the sixties some researchers, including

Leontief, started with using input-output tables to analyse environmental issues, until the creation of environmentally-extended input-output analysis (EEIOA) [59]. While the process analysis based LCI can be regarded as a bottom-up approach, the EEIOA is a typical top-down approach. A process-based LCI is usually modelled through process network analysis, where the product system is broken down into “branches” of processes. In contrast, an input-output LCI model relies on matrix notation. The process analysis is focused on following the chain of production to build the life cycle of a product, while the focus of input-output analysis is on macroeconomics [60].

The advantage of using input-output analysis stands in the possibility to consider the whole economy in the system under study, providing a high degree of completeness. However, while the problem of truncation is avoided, the system analysed lacks the typical level of detail of process analysis, which results in another problem: the aggregation error. Indeed, input-output data are usually aggregated at the economic sector level, which can include a large variety of products, since it is not viable in practice to manage process-specific data for the entire economy. Furthermore, input-output data are commonly available in monetary units, representing economic interindustry transactions. In a context of EEIOA, this implies the assumption that monetary flows are a good representation of the physical flows within an economy, while in practice it is possible that price inhomogeneities distort physical relationships [59].

In the attempt to overcome main limitations of both approaches and preserve at best their strengths, hybrid methods have been developed. Several types of hybridisation can be found in literature, which result in a wide spectrum of methods in which process and input-output analysis represent the two ends. Precisely, four types of hybrid methods have been identified: (1) tiered; (2) path exchange (PXC); (3) matrix augmentation; (4) integrated [59].

Hybrid LCA typically combines process-based LCA in the detailed foreground system and IO-based data as a more generic background system, to benefit both of the process specificity of the LCA and the complete system boundaries of IO analysis. This compromise has been recognised as a more accurate approach than process-based LCA [60] [61], although some criticism on the conceptual superiority exists [62] [63]. The main argument in favour of Hybrid LCA is that completing system boundaries is a fundamental aspect of LCA [64], while the model linearity is usually called into question against it [65]. Remarking upon this latter aspect, *Yang & Heijungs (2019)* [65] suggest rethinking the direction of Hybrid LCA and recommend incorporating other models into LCA, such as system dynamics and econometric models, to compensate for the linear assumptions.



### 1.5.3 Dynamic LCA

A commonly shared definition of Dynamic LCA can hardly be found in literature. However, the most popular definition is the one provided by *Collinge et al. (2013)* [66]: “an approach to LCA which explicitly incorporates dynamic process modeling in the context of temporal and spatial variations in the surrounding industrial and environmental systems”. Correspondingly, the same authors propose their dynamic approach to LCA, realised through the use of the conventional computational structure of LCA in matrix notation [67] for subsequent time steps, and the eventual summation of the impacts:

$$\text{(Equation 1)} \quad \mathbf{h} = \sum_{t_0}^{t_e} \mathbf{C}_t \times \mathbf{B}_t \times \mathbf{A}_t^{-1} \times \mathbf{f}_t$$

Where:

- $\mathbf{h}$  is the impact vector, representing total environmental impacts of the studied system.
- $\mathbf{f}$  is the demand vector, representing the output flows generated for the specific function of the studied system.
- $\mathbf{A}$  is the technosphere matrix, whose inverse multiplied by  $\mathbf{f}$  gives the supply vector  $\mathbf{s} = \mathbf{A}^{-1} \times \mathbf{f}$ , representing all the input flows needed to produce the outputs in the demand vector.
- $\mathbf{B}$  is the biosphere matrix, describing the exchanges with the environment (emissions and resource consumption) associated with the output unit; the product of  $\mathbf{B}$  by  $\mathbf{s}$  gives what is called the LCI.
- $\mathbf{C}$  is the matrix of characterisation factors, which represent the magnitude of the effect of each quantity of emission or resource consumption in each impact category; it can be simplified into a diagonal matrix, assuming that each element of the inventory has effects on a single impact category.
- $t$  represents a point in time at which the values in the various terms are known.
- $t_0$  and  $t_e$  represent the beginning and ending time points of the analysis, respectively (usually the beginning and end of the product or system life cycle).

This approach allows to evaluate time variability distinguishing each component, taking into account different types of potential changes:

- changes associated with the quantities of products needed to perform the system function ( $\mathbf{f}_t$ );
- changes in technological processes ( $\mathbf{A}_t$ );
- changes in unit emissions or unit resource consumptions as a result of changes in technology or regulations ( $\mathbf{B}_t$ );
- changes in background environmental systems affecting fate, exposure and effects dynamics ( $\mathbf{C}_t$ ).

Practically, this approach requires to consider different data sets over a time horizon (e.g. 10 years), each with a specific time duration (e.g. one year) over which a classical LCA computation can be performed. In this way the basic structure of the model is not affected, being still simplified in a linear one but with time differentiation in addition. However, a stricter application of their definition (“an approach to LCA which explicitly incorporates dynamic process modelling”) would imply the dynamic modelling of all unit processes, with a discrete time of operations, accumulation terms and possible time lags between different processes. This model development would dramatically increase the computational complexity, which is not necessary worth the effort. Nevertheless, some promising attempts in this direction are worth to be mentioned.

For instance, *Tiruta-Barna et al. (2016)* [30] try to reach a higher temporal resolution considering supply and demand dynamics of unit processes to model life cycle networks, which results in computing a time dependent LCI though a graph search algorithm. They describe their method as “a journey back in time”, and the problem of loops, typical of network analysis, is solved fixing a back-time horizon (i.e. a time threshold in the past), equivalent to a cut-off rule based on time. However, this method appears as a literal application of the attributional approach, with all its flaws.

Indeed, it can be said that the choice of the attributional or consequential approach has important implication on the consideration of time in the model; according to the definition of *Weidema (2014)* [20] the temporal aspect emerges clearly:

- *An attributional product system is composed of the activities that have contributed to the production, consumption, and disposal of a product, that is tracing the contributing activities backward in time (which is why data on specific or market average suppliers are relevant in such a system).*
- *A consequential product system is composed of the activities that are expected to change when producing, consuming, and disposing of a product, that is, tracing the consequences forward in time (which is why data on marginal suppliers are relevant in such a system).*

It is obvious that only tracing cause-effects relationships forward in time makes sense, according to the principle of temporal precedence of causes [68]. If LCA is regarded as a “journey back in time” starting from the foreground process, it becomes of limited use, at least as a supporting tool for decision-making, which is by definition future-oriented. This turns out to be another argument in favour of the adoption of the consequential approach whenever possible, which is closer to real world dynamics. In this case, assigning emissions occurred in the past to products produces today, just because the production of the physical inputs precedes the production of outputs (from a strictly technical viewpoint), would be less realistic than assuming all emissions at a present point in time.

Instead, from a consequential (and economic) perspective, an additional demand for a product generally causes (and, hence, precedes) an additional supply of its inputs. If time is included in the model for the process modelling of the LCI, a “journey forward in time”, starting from the decision analysed, would be appropriate.

More often, attempts to develop a dynamic LCA do not have the general purpose of including time in the analysis, rather they have a focus on specific issues in which time is particularly relevant. For instance, *Zimmermann et al. (2014)* [69] developed what they call a “time-resolved LCA” for the assessment of electric vehicles, which is not meant to obtain a time-dependent LCI, but to take into account the variation of the electricity mix over the long use-phase of the electric vehicles. Indeed, recognising the importance of the energy transition for many types of products necessarily involves the use of dynamic approaches. Other studies also focus on the electricity consumption for the use phase, but with the purpose to consider the fluctuations in the mix, considering monthly or even hourly resolution. For instance, *Collinge et al. (2018)* [70] assessed the use phase of a building and compared static and dynamic models, exploring variations in both temporal resolution and LCA modelling principles (in particular, the consideration of average electricity mix according to the attributional approach, and marginal electricity generation following the consequential approach); they ultimately showed that the results can change consistently among different models.

The topic of electricity is explanatory for signalling that often two different needs in the context of LCI models are present, that potentially require different tools: on one hand, time is relevant for capturing future structural changes; on the other hand, it is important for considering possible fluctuations of flows over time. To avoid confusion, when the first issue is addressed it is better to refer to the assessment as “prospective”, although the term dynamic is unavoidable and still appropriate in the particular description of the analysis. In the first case, the use of scenarios is relevant, while in the second case the modelling challenge lies in capturing the temporal resolution of the LCI.

# 2 Sustainability of future biorefineries

## 2.1 The biorefinery concept

Among the strategies for the reduction of dependence on fossil fuels and for climate change mitigation, technologies for the conversion of biomass into replacements of current fossil-based products definitely play an important role. Indeed, while the range of renewable sources from which to produce heat and power is quite large (solar, wind, hydro etc.), only biomass can be converted into products with the same function as that of their non-renewable counterparts, including transportation fuels and chemicals [71]. Indeed, besides fossils, biomass is the only C-rich material source largely available at global scale [72].

Consistent with this view, biorefineries draw inspiration from the petrochemical concept of “refinery”, aiming at the development of sequential processes for the transformation and valorisation of organic matter into a set of products suitable for various uses, from production of heat and power, to usage as biofuels in the transport sector, or as chemical compounds of interest for a number of different industrial fields. Such synergistic production has the potential to reach high efficiency in terms of economics, energy and resource use [73]. As a consequence, biorefining is considered the optimal strategy for large-scale sustainable use of biomass in the bioeconomy [74].

## 2.2 The role of bioenergy

Today, biomass use for energy purposes (bioenergy) is the largest global contributor (70%) to renewable energy, accounting for roughly one-tenth of world total primary energy supply, which is

yet dominated by fossil sources [75]. Heat is still the largest sector of final bioenergy consumption (75%), but in recent years bioenergy for electricity and transport biofuels has been growing quickly [76]. While renewable electricity can be also obtained cost-effectively from wind and solar, biomass-based fuels (bioethanol, biodiesel etc.) are considered one of the best options for replacing fossil oil in the transport sector [74]. Indeed, biofuels are the only renewable resources that can reduce in the short term the heavy dependence on fossil oil, without replacing the vehicle fleet. In particular, among biofuels, advanced hydrocarbon biofuels (often referred as drop-in fuels) would have the appealing advantage that they are compatible with existing infrastructure, in terms of tanks, pipelines, pumps, vehicles, and engines, since they are essentially identical to their existing petroleum counterparts in properties, except that they are derived from biomass sources [77].

Nevertheless, the actual share of biofuels in the transport sector is still below 4% [76] and decarbonisation of transport fuel is still problematic.

The main feedstocks for bioenergy are biomass residues from forestry, agriculture, and municipal waste. Differently from biomasses cultivated on purpose, residues and waste have the advantage of avoiding competition for prime cropland. A residual biomass can be defined as “*a biomass that has been generated as a consequence of a human or animal activity but has not generated any economic value in the context in which it has been produced and can therefore be valorised*” [78]. However, alternative uses of residues besides those energy-related need to be considered, for example agricultural residues can be applied on the soil and have a fertilising function [79]. A fair sustainability assessment of a biorefinery should take into account the actual alternative uses of biomasses used as feedstock.

## **2.3 Key issues in the LCA of biorefineries**

The growing interest for biorefineries is accompanied by a growing need for tools capable of capturing the environmental gains of these new solutions as they enter the technosphere, in order to understand to which extent they can have a role for future sustainability targets. In addition, different system setups and process pathways could be feasible and are worth being chosen also on the basis of their overall environmental performance. Life cycle assessment can be considered as the most appropriate methodology to reach this scope; as evidence of this, many LCAs of biorefinery systems have been performed in recent years. However, from a closer look at the studies which have been performed to date, it is clear that key methodological issues in the framework of LCA analysis are

still far from reaching a consensus, while having at the same time a high influence on the results of the analysis. It can be affirmed that bioenergy in particular poses more methodological challenges than other types of energy [80].

The literature on the topic has been reviewed in previous studies [73] [81], that have contextually discussed the issued related to the main methodological choices. One important premise is that these choices are in any case strictly connected to the specific objective of the study. Indeed, the research aim can be essentially of three types:

- A. *Use of feedstock*: to assess the environmental benefits of using a biomass in a biorefinery system against alternative uses of the biomass;
- B. *Production of a specific product*: to assess the environmental benefits of producing a certain product within a biorefinery system against alternative conventional processes for its production;
- C. *Biorefinery as a whole*: to assess the environmental benefits of building and running a biorefinery compared with business as usual and/or studying the optimal setup for process configuration that minimize environmental impacts and/or identifying hotspots of environmental impacts.

### 2.3.1 Functional unit and the multifunctionality problem

First of all, the goal of the study has an effect on the choice of the functional unit, which should reflect the function of the systems that are object of comparison.

An input based functional unit is requested for situations of the type A, while an output based functional unit is needed for situations of the type B. In the first case, the function of the biorefinery is related to the biomass use, and the system providing the best use for biomass has to be sought; for example, a biorefinery using wood as a feedstock can be compared to traditional systems that burn the biomass to produce energy or that use it in manufacturing processes for wood products. This applies also to the case of a waste biomass, in which the biorefinery is regarded as a valorisation strategy to be compared with other ways to manage the waste (e.g. landfilling, incineration). In the second case, the focus is on the (main) product, therefore the function is its production; a typical example is biofuel, therefore the biorefinery can be compared with a traditional refinery providing a fossil-based fuel. To take into account possible different physical characteristics of the two types of fuels, which can result in different engine conversion efficiencies, the functional unit can be moved from a physical property (e.g. 1 kg of fuel) to the energy content (e.g. 1 MJ of fuel), or – more appropriately – to the one expressing the very function of the product, which in the specific case

would be “driving” (e.g. 1 person-km). However, biorefineries by definition produce more than one product and the use a multifunctional unit is more appropriate for situations of type C. Therefore, a combination of output products (e.g. 1 MJ of biofuel *and* 2 kg of bioplastic *and* 0,5 MJ of electricity) or the whole biorefinery system (e.g. 1 biorefinery) can be regarded as the functional unit. The disadvantage of this choice is that the aggregated results limit the possibility of comparison with other studies. On the other hand, there is a clear advantage in this choice, since in the system to be analysed the multifunctionality problem is avoided: in practice, this situation corresponds to a system expansion for the system to be compared with the biorefinery system. In this regard, it is important to clarify that *system expansion* (or “*system enlargement*”) is mathematically equivalent to *substitution* (also called “*crediting*” or “*avoided burden approach*”), although being conceptually different, as specified in the ILCD Handbook (p.77) [21]. Indeed, they can be regarded as the two faces of the same coin, and for this reason are often confused. The difference is illustrated in Fig. 4. “Substitution” refers to a situation in which the functional unit is related to a product X, and Y is a possible co-product; the biorefinery system, in order to be compared to another system with the same function (i.e. producing X), includes the avoided impacts due to the substitution of the alternative system producing Y. “System expansion” refers to a situation in which the functional unit includes both the production of X and Y, hence the biorefinery system is compared with a combined system of two alternative systems, producing X and Y respectively.

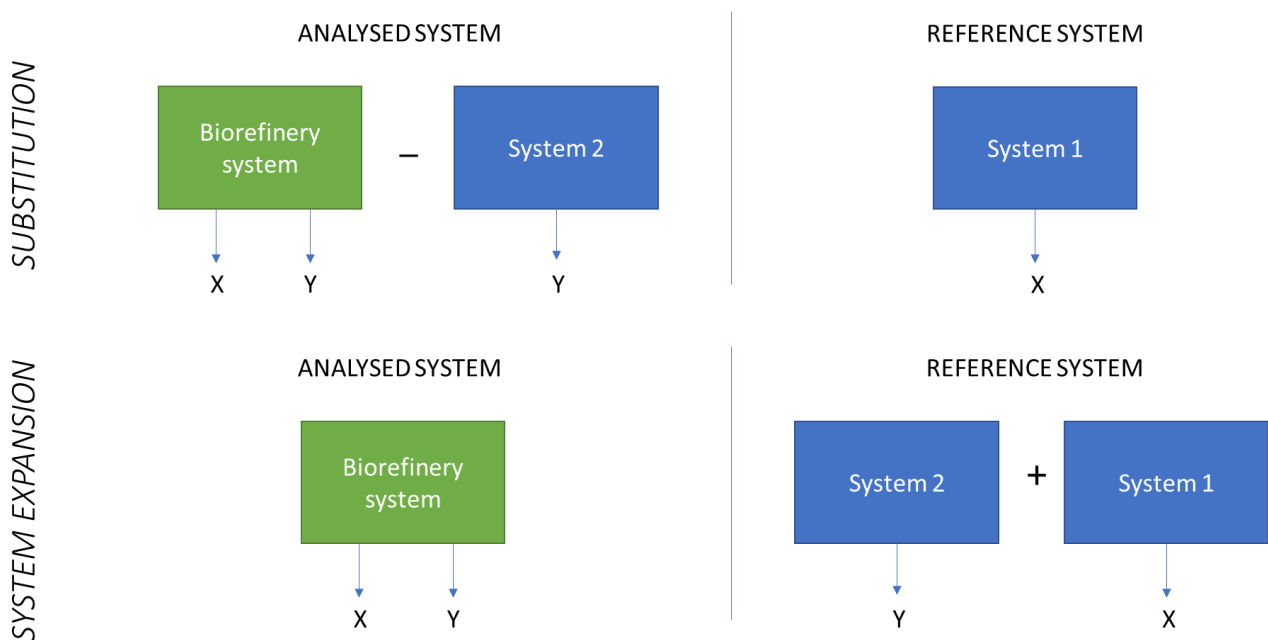


Fig. 4 – Illustration of substitution and system expansion methods.

Substitution can be applied to situations of type A and B, in which the system analysed does not involve all functions provided by the biorefinery and a multifunctionality problem has to be addressed. Both system expansion and substitution require to identify the alternative systems providing the same functions, commonly consisting of systems producing fossil-based goods. In some cases, the identification of the alternative system is straightforward, for example when the product is a biofuel, heat or electricity. However, for some products that fulfil a more complex function, such as nutritional or pharmaceutical, or that might have novel attributes, it could be difficult to identify the alternative system fulfilling the same function. Moreover, additional data are required to include alternative systems in the analysis. Therefore, when the correct identification of alternative systems is not possible or too difficult, *allocation* can be applied: this procedure consists in “partitioning the input or output flows of a process or a product system between the product system under study and one or more other product systems” [17]. In practice, the product system (i.e., in this case, the biorefinery system) is virtually cut in portions attributed to each function of the system, and all portions not referring to the studied function are taken out from the analysis. An illustration is provided in Fig. 5: “allocation” refers to a situation in which the functional unit is related to a product X, and Y is a possible co-product; the biorefinery system, in order to be compared to another system with the same function (i.e. producing X), is partitioned in two fractions, one attributed to product X and one attributed to product Y, which is left out of the analysis.

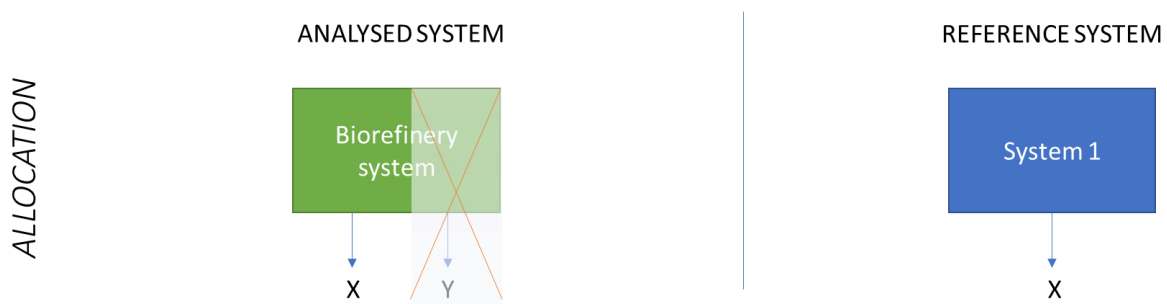


Fig. 5 – *Illustration of allocation method.*

Allocation can be based on physical properties (e.g. mass or energy) of the products when there is a close correlation between the chosen physical property and the value of each product. Often this is not possible for a biorefinery, since some products can have an energy value and other products not, for example a biorefinery producing fuels/heat/electricity and fine chemicals with a non-energy related function. For this reason, the economic value of each product seems a more appropriate allocation criterion. Indeed, economic allocation based on market value is the most common procedure for allocation in LCA for several different production sectors, including biofuels sector



[81] [82]. Nevertheless, economic allocation is regarded as the last option in the hierarchy for allocation defined by the ISO standards. The main complication in referring to the economic value is its transient nature, due to price fluctuations. In order to minimise this problem, expected revenue has been proposed for economic allocation [82], since it fluctuates less over time than actual prices; after all, economic profit from a system is one of the reasons it exists.

Finally, it should be noted that the ISO standards suggest in the first place to try to avoid allocation by increasing the level of detail of the system, a method indicated in the ILCD Handbook as “*subdivision*”. However, many processes in a biorefinery are impossible to divide into sub-processes, thus the multifunctionality would not be eliminated completely. Furthermore, even when sub-processes can be modelled as physically separated, they could still depend on each other, for example because the economic viability of the whole system relies on that specific combination of processes [83].

A particular issue is posed when biomass waste or residues are used as feedstock. Indeed, if the input of a biorefinery has a negative economic value, i.e. the biorefinery is paid to accept it, waste treatment should be considered as one of the functions of the biorefinery. In this case, the function is not associated with a product output but to an input used by the system. For this reason, it would be recommendable to refer more generally to “functional flows” and not to products, intending the flows associated with a function of the system, regardless of whether they correspond to physical outputs or inputs. From an economic perspective, functional flows always correspond to positive economic inputs (i.e. the system is paid to provide its functions to other systems), while the non-functional flows (with the exception of environmental elementary flows, hence only the intermediate flows) correspond to positive economic outputs (i.e. the system pays for functions provided to it by other systems). Therefore, if a waste flow is managed by the biorefinery system, the alternative system that would manage the waste should be identified if substitution or system expansion is applied, while economic value could be a good criterion if allocation to the co-function of waste management is chosen to deal with multifunctionality. However, a clear distinction between products and wastes, based on the economic value of flows, is not always possible. For example, someone may pay to have their residues picked up, while someone else pays to receive it. Shifts from positive to negative prices for this type of goods can happen through time and space, due to market fluctuations, technological developments and policy regulations [80].

### 2.3.2 Land use and biogenic carbon

More specific issues concern the consideration of land use and biogenic carbon.

Any biorefinery involves by definition the use of biomass, which is generally connected to some form of land use. A distinction is usually made between land use and land use change, and the latter in turn is divided in direct and indirect land use change. In brief, land use refers to the occupation of land for a certain time, maintaining the state of land altered from the one that would be there otherwise; instead, land use change refers to the transformation of land with respect to a previous state or, more extensively, a change in the properties of the land surface area. While land use is distributed over time, land use change *happens* at a single point in time (although its effect can still be distributed over time) [84]. With reference to a biorefinery project, direct land use change would involve changes in the site used for feedstock production, whereas indirect land use change refers to changes in land use that would take place elsewhere as a consequence of the biorefinery project, through market-mediated effects [85]. There is a certain agreement on the importance of the inclusion of land use and land use change in LCA, though the debate on how to include them in the framework remains quite open: sometimes they are regarded as activities, sometimes as inventory items, other times as impacts [80]. It could be said that biorefinery does not entail land use issues when waste sources are used. However, if these biomass sources were previously used for other purposes, land use change effects can still arise. For example, if harvest residues were left in the field, their alternative use in a biorefinery could result in decreasing soil productivity and lower yields, eventually increasing the need for new land to compensate for lost production [85].

For what concerns biogenic carbon, it is often assumed that carbon dioxide emissions from biomass are climate neutral. However, this can be true only when the emission of biogenic carbon due to the biorefinery facility is really compensated by an equivalent amount of photosynthetic carbon sequestered by naturally grown vegetation, i.e. the biomass feedstock should be produced in a sustainable way, assuring that the natural regeneration capacity is not overcome. Another complication could originate from the possibility that part of the carbon stored in the biomass is not released as CO<sub>2</sub> but as CH<sub>4</sub>, a much stronger greenhouse gas, e.g. due to a process of incomplete burning or anaerobic decomposition with leakages occurring along the way. On the other hand, if there is a significant time lag between the uptake and release of biogenic CO<sub>2</sub> in the studied system, credits associated to carbon storage or delayed emissions could be considered [86].

### 2.3.3 ALCA vs. CLCA

The goal of the study is decisive also for choosing between an attributional or consequential approach, which in turn determines most of the methodological choices on the above reviewed issues. However, when performing ALCA or CLCA (depending on the research goal), and how to apply ALCA or CLCA (methodological choices implied by the approach) are questions still debated in the scientific community; as a consequence, the distinction of the two approach do not solve the methodological issues but add up to the inconsistencies among studies.

Biorefineries, and particularly bioenergy options, are often meant to be implemented at large scale. In this type of situations, CLCA seems more appropriate, since results would depend on the actual magnitude of the implementation, and not linearly dependent on the functional unit.

# 3 Case study: TCR-PSA-HDO system

## 3.1 Technology description

An example of biorefinery is offered by the system currently investigated in the European H2020 project “The demonstration of waste biomass to Synthetic Fuels and Green Hydrogen – TO-SYN-FUEL” [87]. The project runs from 2017 until 2022 and is implemented by twelve partners from industry and academia from five European countries. The ambition of this project is to demonstrate the technical and economic viability, as well as the environmental and social sustainability, of a new integrated process which combines Thermo-Catalytic Reforming (TCR©) [88], a thermochemical process of biomass conversion developed by Fraunhofer UMSICHT, with hydrogen separation through pressure swing adsorption (PSA), and hydro-deoxygenation (HDO). The integrated process enables the production of a fully equivalent gasoline and diesel substitute (compliant with EN228 and EN590 European Standards) and green hydrogen for use in transport. In respect of the proven pilot scale TCR concept, the project aims to validate and demonstrate the combined technology at near commercial scale, with an advancement from TRL-5 to TRL-7.

Such technology utilises sewage sludge as feedstock, a problematic organic industrial waste which today is largely disposed of by incineration, landspreading or landfilling [89]. Sewage sludge from waste water treatment plants has a high water content (>95%), therefore it has to be subjected to pre-treatment in order to remove most of the aqueous component, before being sent to the thermochemical process in the TCR plant. The latter consists of a pyrolyser operating at intermediate temperatures (350-500 °C) followed by a catalytic reformer: in the first stage the biomass is decomposed thermally in biochar and volatile compounds, while in the second stage the catalytic properties of the biochar product itself are exploited, so that it is mixed again and placed in contact with the volatile compounds at a higher temperature (650-700 °C), thus determining their upgrading into high quality gas and oil

for fuel. From the synthesis gas it is possible to obtain pure hydrogen through the PSA technology, which is based on selective absorption by certain materials at high pressure with respect to compounds contained in a gaseous stream, and subsequent desorption at low pressure. Hydrogen thus obtained is partially used in the process for the oxygen removal (HDO), to which the oils in output from the TCR are subjected to, acquiring this way the features that will render them suitable for direct use in common transport engines (diesel and gasoline). The final separation of the HDO oil into sellable products requires a distillation step. The char and the residual fraction of syngas may instead be used for the production of heat and power, thus satisfying the internal energy demand of the whole process and providing most of the thermal energy required by the dryer, while excess electricity can be sent to the grid. After gasification, the resulting ash is a waste product rich in phosphorus, which is eventually recovered through extraction with sulphuric acid. A process flow diagram of the integrated process is provided in Fig. 6.

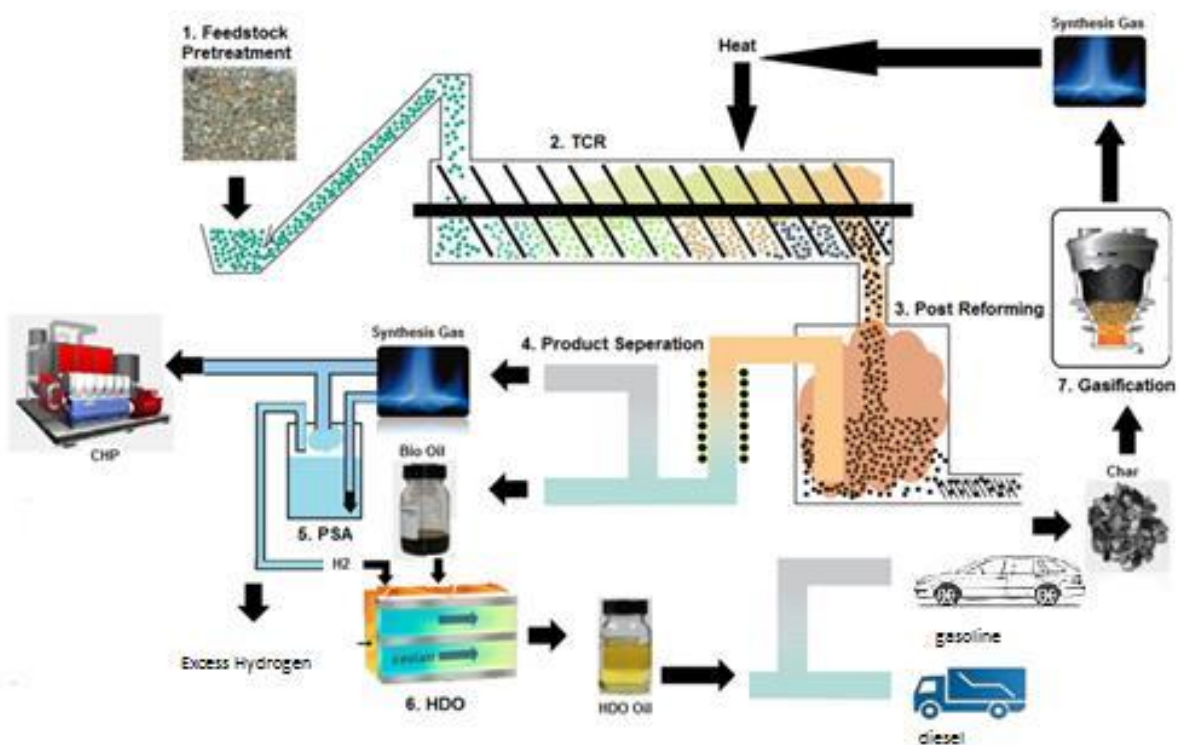


Fig. 6 – Process flow diagram of the integrated TCR-PSA-HDO process

## 3.2 LCA of the TCR-PSA-HDO system

The validation of the integrated technology at larger operational scale includes all social, environmental and economic aspects. In particular, Work Package 6 of the project aims at quantifying the environmental sustainability of the integrated TCR-PSA-HDO technology, through sustainability metrics including LCA, GHG, mass and energy balance, comparing its performance against alternative technologies and feedstock valorisation routes in support of a subsequent commercialisation.

A conventional LCA, compliant with ISO standards, has been set in the project. The primary data collected of the TCR-PSA-HDO integrated system were referred to a plant size of 500 kg/h (10% water content) of feedstock processed. The operating time of the plant have been set at 7000 h/year.

Two separate goals have been identified and different system boundaries, functional units have been defined accordingly:

1. ‘process oriented’: to assess the environmental benefits of the new technology as new alternative for “end of life” of the feedstock used;
2. ‘product oriented’: to assess the environmental performance of the new technology versus the current technologies that it replaces.

Methodological choices for each goal are shown in Tab. 1.

Tab. 1 – *Methodological choices for the LCA approaches in the conventional framework*

<b>Approach</b>	<b>Function</b>	<b>Functional unit</b>	<b>Multifunctionality handling</b>	<b>Alternative scenarios</b>
Process oriented	Sewage sludge management	1 tonne of sewage sludge ready to be treated (water content: 98 %w/w)	Substitution	○ LAND SPREADING ○ INCINERATION ○ LANDFILLING
Product oriented	Fuel production	1 MJ of higher heating value in the produced fuel	Energy allocation for gasoline and diesel. Substitution for possible credits by hydrogen, phosphorous, electricity.	CONVENTIONAL GASOLINE and CONVENTIONAL DIESEL

In both cases, start-up, shut-down and maintenance, emergency flows and fugitive emissions, and capital goods (e.g. construction of factory buildings, vehicles, machines and auxiliary equipment) were not included. The required additional heat has been assumed to be supplied by natural gas. The organic matter in sludge was assumed to be entirely biogenic, thus CO<sub>2</sub> emissions associated with combustion of the syngas and biochar were not included.

### 3.2.1 Inputs and outputs of the foreground system

The analysis of the foreground system involved data collection and calculation procedures to quantify relevant inputs and outputs of the specific TCR-PSA-HDO combined technology. A schematic representation of the processes included in the system and the main flows among them is provided in Fig. 7.

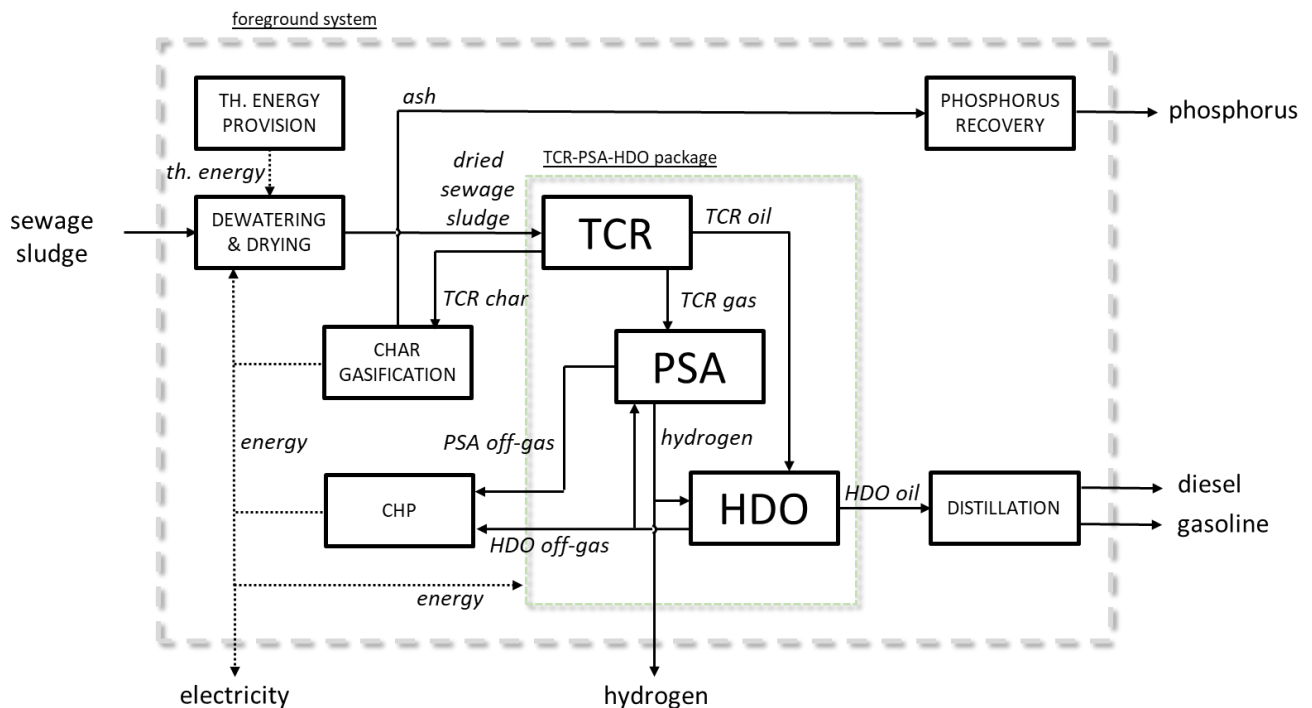


Fig. 7 – Foreground system of the TCR-PSA-HDO technology

Tab. 1 lists inputs and outputs by each unit process considered in the model for the foreground system. The following notation has been adopted: intermediate flows are indicated in bold, while simple notation is used for elementary flows; flows exchanged between processes in the foreground system are in italics; intermediate flows crossing the boundaries of the foreground system are underlined>. It should be noticed that the latter are always associated to functions provided by the system.

Tab. 2 – Process units and main input and output flows identified for the foreground system

process	flow	I/O	u.m.
DEWATERING & DRYING	<b><u>Sewage Sludge (98% w/w)</u></b>	I	kg
	<b>Electricity</b>	I	MJ
	<b>Thermal energy</b>	I	MJ
	<i>Sewage Sludge (10% w/w)</i>	O	kg
	Water vapour	O	kg
TCR	<i>Sewage Sludge (10% w/w)</i>	I	kg
	<b>Electricity</b>	I	MJ
	<b>Thermal energy</b>	I	MJ
	<b>Nitrogen</b>	I	kg
	<b>Lubricating oil</b>	I	kg
	<b>Softened water</b>	I	kg
	<b>Cooling water</b>	I	kg
	<i>TCR oil</i>	O	kg
	<i>TCR gas</i>	O	kg
	<i>TCR char</i>	O	kg
	<b>Process water</b>	O	kg
	<b>Thermal energy (recovered)</b>	O	MJ
	PSA	<i>TCR gas</i>	I
<i>HDO off-gas</i>		I	kg
<b>Electricity</b>		I	MJ
<b>Nitrogen</b>		I	kg
<b>Compressed air</b>		I	Nm3
<b>Activated coal</b>		I	kg
<i>PSA off-gas</i>		O	kg
<b><u>Hydrogen</u></b>		O	kg
<b>Activated coal</b>		O	kg
HDO	<i>TCR oil</i>	I	kg
	<i>Hydrogen</i>	I	kg
	<b>Electricity</b>	I	MJ
	<b>Nitrogen</b>	I	Nm3
	<b>Compressed air</b>	I	Nm3
	<b>Steam</b>	I	MJ
	<b>Tap water</b>	I	kg
	<b>Catalysts</b>	I	kg
	<i>HDO oil</i>	O	kg
	<i>HDO off-gas</i>	O	Nm3
	<b>Process water</b>	O	kg
<b>Catalyst (waste)</b>	O	kg	



Tab. 2 – (continued)

process	flow	I/O	u.m.
DISTILLATION	<i>HDO oil</i>	I	kg
	<b>Electricity</b>	I	MJ
	<b>Thermal energy</b>	I	MJ
	<u>TSF Diesel</u>	O	kg
	<u>TSF Gasoline</u>	O	kg
CHAR GASIFICATION	<i>TCR char</i>	I	kg
	<i>Ash</i>	O	kg
	<b>Electricity</b>	O	MJ
	<b>Thermal energy</b>	O	MJ
CHP GENERATION	<i>PSA off-gas</i>	I	kg
	<i>HDO off-gas</i>	I	kg
	<b>NaOH</b>	I	kg
	<b>H<sub>2</sub>SO<sub>4</sub></b>	I	kg
	<b>Lubricating oil</b>	I	kg
	<b>Water</b>	I	kg
	<u>Electricity</u>	O	MJ
	<b>Thermal energy</b>	O	MJ
	NO <sub>x</sub> emissions	O	kg
N <sub>2</sub> O emissions	O	kg	
PHOSPHORUS RECOVERY	<i>Ash</i>	I	kg
	<b>Electricity</b>	I	MJ
	<b>Steam</b>	I	kg
	<b>HCl</b>	I	kg
	<u>Phosphorus</u>	O	kg
	<b>Waste (ash)</b>	O	kg
THERMAL ENERGY PROVISION	<b>Natural gas</b>	I	Nm <sup>3</sup>
	<b>Thermal energy</b>	O	MJ
	CO <sub>2</sub> emissions	O	kg

### 3.3 Future targets for market deployment

The ambition of the project is, following the demonstration phase at TRL-7, to open the way for the scale up of the technology to commercial scale. Key performance indicators have been established both within the project and for deployment on a wider European scale. It is estimated that the first flagship plant processing at least 3 t/h of low-moisture biomass could be fully installed and commercially operational by 2022, with roll out of at least 50 commercially operating plants established by 2030. Based alone on the available amount of produced sewage sludge and taking into consideration that TCR/PSA/HDO plants can be economically operated at a variety of scales in both centralised and decentralised modules, a further adoption of the process up to 300 TCR units by 2050 is targeted. It is estimated that the maximum size of such a type of facility could process up to 40 t/h of low moisture biomass into renewable energy, transport fuels and green chemicals. By doing this, this technological system aims to contribute towards significant GHG savings and diversion of organic wastes from landfill.

Tab. 3 – *Targets for future market deployment in European Union*

year	target	
	number of plants	production capacity
2030	50 plants	3 t/h
2050	300 plants	3 t/h up to 40 t/h

### 3.4 How to assess the biorefinery system beyond the conventional LCA framework? A proposal

The conventional LCA of the biorefinery associated to the TCR-PSA-HDO technology, presented in section 3.2, falls into the categories A and B of studies described in section 2.3.1. More precisely, the process-oriented approach corresponds to type A, analysing the use of sewage sludge feedstock against alternative management options, whereas the product-oriented approach corresponds to type B, assessing the production of fuels against conventional processes for their production. However, from the review of LCA for biorefineries emerged that a third approach can be followed, which consists in evaluating the biorefinery as a whole. This approach can be suitable for answering to

different research questions, such as assessing the environmental benefits of building and running a biorefinery compared with business as usual. Therefore, the focus of the assessment will not be on specific functions anymore, but on the decision of building and running the biorefinery and its environmental consequences. A change-oriented (or consequential) perspective is typically needed in these situations. Furthermore, the actual magnitude of the technology implementation can be relevant and should be considered in the analysis. Finally, the targets for future market deployment of the TCR-PSA-HDO technology, presented in section 3.3, are medium to long-term goals, while especially the field of bioenergy is rapidly evolving towards a structurally different global scenario. For this reason, it would be also appropriate to evaluate the technology with a prospective assessment with dynamic components.

Based on these considerations, the research question is formulated as follows:

***What is the environmental impact of the decision to implement the biorefinery system associated to the TCR-PSA-HDO technology in Europe (compared with business as usual), according to the targets for commercial deployment expected in the TSF project?***

In the wake of the recent developments in LCA modelling discussed in section 1.5, the present study is performed proposing a modelling approach presented in the next chapter. It includes a dynamical long-term perspective, relies on IO analysis for expanding the system boundaries to all sectors of the economy, and is designed for capturing the broader environmental consequences following a consequential approach.

# 4 Proposed modelling approach

## 4.1 General framework

The proposed advanced LCA framework has the structure depicted in its salient steps in Fig. 8, where it is compared to the conventional LCA framework.

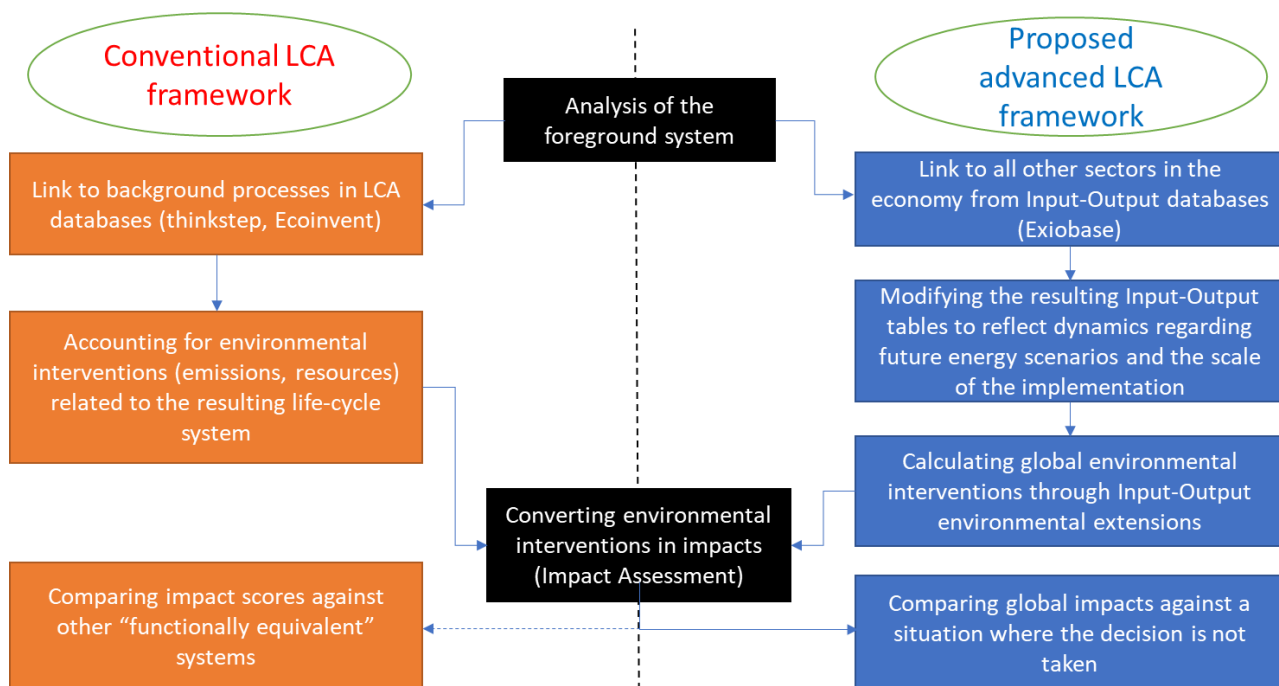


Fig. 8 – General framework for the proposed advanced LCA compared to the conventional LCA

The study starts in both cases from the analysis of the foreground system (black box in the upper part of the figure). After that, a classical LCA (left part of the figure) would then expand the system boundaries including background processes associated with the intermediate flows or to the co-functions. These processes are usually retrieved by LCA databases (e.g. Thinkstep or Ecoinvent), and

represent activities which are assumed to fulfil the demand in the foreground system associated with the intermediate flows, or which will substitute the co-functions provided by the system, when substitution is chosen as the method to handle multifunctionality. In this way, the starting system becomes the core part of a wider supply chain and can be studied in a life cycle perspective. Instead, in the proposed framework (right part of the figure) the foreground system is englobed in a technological matrix representing all sectors of the economy, and it is regarded as being a component of the whole economic system. The technological matrix is derived from input-output tables (IOTs) available in IO databases (e.g. Exiobase). The following step consists in the modification of the matrix, in order to reflect dynamics regarding both future technological scenarios and the scale of the implementation of the studied technology englobed in the economic system. This results in a dynamic framework in which the scale of the novel technology can change over time and can be evaluated in a changing context. Subsequently, global environmental interventions (emissions, resources) are calculated using environmental extensions provided in IO databases, which associate a certain amount of input and outputs from and to the environment to the operation of each economic sector. By doing this, it is possible to obtain the inventory of the global economic system, whereas the conventional LCA aims to obtain the life cycle inventory associated to the specific product system. Similarly to what would be done for a conventional LCA, the subsequent step consists in the characterisation phase of the LCIA, in which the inventory of environmental interventions is translated in impacts through the use of characterisation factors. In the proposed framework, a final step is required, since calculated global impacts have to be compared to those obtained in a “no decision” scenario, i.e. a situation in which the operation of the global system is simulated without the studied technology. The comparison is thus capable to provide the global changes to be attributed to the decision and ultimately its environmental consequences. It should be noticed that, in the proposed framework, the assessment involves a comparison in itself, while a conventional LCA would assess the impacts related to a product life cycle to be compared subsequently with other systems which are assumed to provide the same function(s) *ceteris paribus*. Indeed, it can be said that the final results in the conventional framework are absolute values (absolute impacts attributed to a function), while the proposed framework provides relative values (relative impacts attributed to a decision).

The steps for building the model are illustrated in general terms in the following sections of this chapter, while the specific application to the case study is described in the following chapter.

## 4.2 Analysis of the foreground system

First of all, the technology has to be characterised in its inherent aspects, that is to say inputs and outputs of the corresponding foreground system; the latter can be regarded as the starting point to retrace a supply chain for a life cycle analysis.

At this stage, it is important to classify inputs and outputs of the foreground system in the following terms:

- functional flows: inputs and outputs related to functions provided by the system;
- intermediate flows: inputs and outputs related to functions demanded by the system;
- elementary flows: inputs of resources from the environment and outputs of emissions to the environment.

This distinction is essential to prepare the following step, when the foreground system has to be linked to other sectors in the economy. The functional flows represent the direct interaction of the foreground system with other systems in the economy, in terms of functions provided to other sectors; the intermediate flows represent the same type of interaction the other way round, i.e. in terms of functions requested by the system from other sectors. Finally, elementary flows represent the direct interaction of the foreground system with the environment.

If monetary IO tables are planned to be used, physical (and energy) functional and intermediate flows have to be translated in monetary terms. Market information on prices regarding the products exchanged need to be collected to perform this step. In theory, goods' prices can change consistently over time and affect the results of the analysis. Thus, assuming constant prices can be regarded as a strong assumption; however, the interest is not in monetary flows themselves, but in recreating physical flows exchanged in the systems using monetary flows as a proxy. In any case, the inherent uncertainty of prices should be taken into account in an uncertainty analysis.

### 4.3 Input-Output tables and aggregation

Input-output tables (IOTs) are top-down models which are able to provide a representation of the entire economy, reflecting the monetary interdependencies between all industries in the economy of a region. Environmental IOTs also include extensions (so-called *satellite accounts*) reflecting the physical dependencies of these industries on the environment. IOTs are generally compiled at nation level and with reference to a specific point in time (e.g. year 2010). In particular, multi-regional IOTs collect national accounts data to recreate a spatially explicit representation of the complex net of global economy, and are crucial for taking into consideration the role of international trade [6].

In general, a *transaction matrix* is a matrix of which a column represents the inputs of a sector/industry from other sectors/industries, and vice versa a row represents the outputs of a sector/industry to other sectors/industries in the economy.

Multi-regional IOTs describe the global inter-sector flows within and across regions for  $k$  regions with a *transaction matrix*  $Z$ :

$$(Equation 2) \quad Z = \begin{pmatrix} Z_{1,1} & Z_{1,2} & \cdots & Z_{1,k} \\ Z_{2,1} & Z_{2,2} & \cdots & Z_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ Z_{k,1} & Z_{k,2} & \cdots & Z_{k,k} \end{pmatrix}$$

Submatrices of  $Z$  are square matrices of  $n$  dimension, where  $n$  is the number of sectors, therefore  $Z$  results in a square matrix of  $n \times k$  dimension. Each submatrix on the main diagonal ( $Z_{i,i}$ ) represents the domestic interactions for each of the  $n$  sectors, while off diagonal matrices ( $Z_{i,j}$ ) describe the trade from region  $i$  to region  $j$  for each sector.

Accordingly, *global final demand*  $Y$  can be represented by:

$$(Equation 3) \quad Y = \begin{pmatrix} y_{1,1} & y_{1,2} & \cdots & y_{1,k} \\ y_{2,1} & y_{2,2} & \cdots & y_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ y_{k,1} & y_{k,2} & \cdots & y_{k,k} \end{pmatrix}$$

Where  $y$  are vectors of  $n$  elements, therefore  $Y$  results in a matrix of  $n \times k$  rows and  $k$  columns. Demand vectors on the main diagonal ( $y_{i,i}$ ) represent internal demand, while off diagonal vectors ( $y_{i,j}$ ) represent direct import to final demand from country  $i$  to  $j$ .

The global economy can thus be described by:

$$\text{(Equation 4)} \quad \mathbf{x} = \mathbf{Z} \cdot \mathbf{i} + \mathbf{Y} \cdot \mathbf{i}$$

where  $\mathbf{i}$  represents the identity vector (column vector with 1's of appropriate dimension) and  $\mathbf{x}$  the vector of *sector total output* of  $n \times k$  elements.

It is convenient to define a *matrix of technical coefficients*  $\mathbf{A}$  (also “input-output coefficient matrix”, or “direct input coefficient matrix”), which can be obtained multiplying  $\mathbf{Z}$  with the diagonalised and inverted vector  $\mathbf{x}$ :

$$\text{(Equation 5)} \quad \mathbf{A} = \mathbf{Z} \cdot \hat{\mathbf{x}}^{-1}$$

$\mathbf{A}$  results in a square matrix with the same size of  $\mathbf{Z}$ , and can be used to calculate sector total output  $\mathbf{x}$  for any arbitrary vector of final demand  $\mathbf{y}$ :

$$\text{(Equation 6)} \quad \mathbf{x} = (\mathbf{I} - \mathbf{A})^{-1} \cdot \mathbf{y}$$

with  $\mathbf{I}$  defined as the identity matrix with the size of  $\mathbf{A}$ .

A more detailed description of mathematical foundations of IO analysis can be found in Miller & Blair (2009) [90].

A number of initiatives are aimed to compile global multi-regional IOTs, such as World Input-Output Database (WIOD) [91], EXIOBASE [92], EORA [93] and GTAP-MRIO [94]. The choice among the available IOTs can be dictated by the desired level of industry detail, geographic scope and accounting methodologies.

Since big amount of data is involved for matrices of high dimension, it is usually convenient to transform the IOTs available into more manageable forms when used for a specific purpose. For instance, some regions can be aggregated to reduce the dimension of  $\mathbf{Z}$  matrix acting on  $k$  index (i.e. reducing the number of  $k \times k$  submatrices), or some sectors can be aggregated to reduce the  $n$  dimension of  $\mathbf{Z}$  submatrices.

## 4.4 Hybrid LCA with matrix augmentation

Once the new sector has been defined and a model of all sectors in the economy is made available, the following step consists in linking the two components. The technique used for this type of hybridisation between LCA and IO analysis is the matrix augmentation [95], which involves the direct



modification of the input-output matrix to create additional sectors of the economy, where process data are used to simulate the physical requirements of the new sector. This method is particularly suited for hybrid LCA of new or emerging technologies [59].

The augmentation process involves the direct modification of the *matrix of technical coefficients*  $A$ , adding a row and a column for each new product.

Coefficients in the new rows require to introduce some *substitution factors* ( $sf$ ), representing the level of substitution between each new product and their competitive ones, calculated in the following way:

(Equation 7)

$$sf_{S \rightarrow N} = \frac{x_N}{x_S}$$

Where the subscript 'N' refers to a new product and subscript 'S' refers to a substituted product.

The substitution factors are then used to modify the rows of the  $A$  matrix for the new products, as well as the substituted products, in the following way:

(Equation 8)

$$a_{Nj}(1) = a_{Sj}(0) \cdot sf_{S \rightarrow N}$$

(Equation 9)

$$a_{Sj}(1) = a_{Sj}(0) \cdot (1 - sf_{S \rightarrow N})$$

Where '(0)' and '(1)' refer to an initial state (before substitution) and a second state (after substitution), respectively.

This step involves two assumptions:

- 1) The new products provide exactly the same type of functions of other products already present in the economy, i.e. the new products can play the same role of other products in the economy, providing their functions to other sectors in the same way and with already established proportions;
- 2) Perfect substitution applies between new products and substituted products, therefore the following equivalence holds:  $a_{Nj}(1) + a_{Sj}(1) = a_{Sj}(0)$ . In principle, it is possible to modify Equation 9 to model an unperfect substitution by subtracting  $sf_{S \rightarrow N}$  to a number different from the unit.

The same reasoning applies to the *final demand vector*  $y$ , therefore its elements are modified in the following way:

(Equation 10)

$$y_N(1) = y_S(0) \cdot sf_{S \rightarrow N}$$

(Equation 11)

$$y_S(1) = y_S(0) \cdot (1 - sf_{S \rightarrow N})$$

On the other hand, new columns of matrix  $A$  are compiled considering the requirement of the new sector, which can be derived from the analysis of the foreground system. Specifically, intermediate flows are considered and their correspondences with products in the IOTs must be preliminarily established. Since coefficients in the columns of matrix  $A$  refer to inputs per unit of product in the  $j$ -th column, these would be equal to the ratio between the intermediate flows associated with the  $i$ -th product in a row and the functional flow related to the product in the  $j$ -th column. However, since the intermediate flows are not attributed to each specific new product but to the biorefinery sector as a whole, they are calculated with respect to the total revenues of the biorefinery and then weighting factors are used to “allocate” the inputs to each function of the biorefinery sector. This procedure has similarities with a revenue-based economic allocation, however it is not aimed to move some functions out of the studied system, but to fragment the technology into different functions to each of which can be ultimately attributed a portion of the biorefinery impacts.

## 4.5 Dynamic framework and future scenarios

Many structural changes in the economy and the technological systems are likely to occur in the future. Since the environmental performance of a product system can be quite sensitive to its context and other systems’ response in the economy, a dynamic prospective analysis would be more appropriate for measuring the broader environmental consequences of an action which unfolds over a long period of time.

Furthermore, available IOTs are generally several years old [28], e.g. the most recent of the available EXIOBASE IOTs refer to year 2011. These tables should be better updated in order to be used for prospective analysis, assuming certain trends occurring in the sectors of the economy. Any structural change can be modelled modifying technical coefficients in matrix  $A$ . However, predicting future changes is not an easy task. In this case, the focus was on the electricity sector, for which it is clear that important changes will happen in the near future and can be quite easily modelled based on future electricity scenarios.

The classical structure of an IO analysis is thus transferred into a dynamic framework, in which all variables exhibit a dependence on the time step:

$$(Equation 12) \quad \mathbf{Z}_t = \mathbf{A}_t \cdot \hat{\mathbf{x}}_t$$

$$(Equation 13) \quad \mathbf{x}_t = \mathbf{Z}_t \mathbf{i} + \mathbf{y}_t$$

where:

$x$  = sector total output vector

$Z$  = transactions matrix

$A$  = technical coefficients matrix

$y$  = final demand vector

$i$  = identity vector (summation vector)

For each time step  $A$  and  $y$  are given as inputs. Initial values for  $Z$  and  $x$  are given as well, consistent with initial values of  $A$  and  $y$ , while for the subsequent time steps they are recalculated according to the aforementioned formulas. The static IOTs are used to define initial values of all variables.

Matrix  $A$  is modified with the aim to reflect dynamics regarding both future technological scenarios and the scale of the implementation of the studied technology englobed in the economic system.

Vector  $y$  is modified as well, in order to consider future trends in final demand for each scenario.

## 4.6 Comparative impact assessment

The resulting gross output vector  $x$  is then used to obtain the impact vector  $h$ :

$$\text{(Equation 14)} \quad h_t = C \cdot B \cdot x_t$$

where  $B$  is the *matrix of environmental stressors*, which coefficients represent the amount of emissions or resource consumption per unit of each sector output, and  $C$  is the *matrix of characterisation factors*, which represents the contribution of environmental stressors in each impact category considered in the analysis. Coefficients in  $B$  and  $C$  matrices are here assumed static, although in principle this framework would allow for the introduction of time-dependent coefficients. Indeed, a dynamic matrix  $B$  would take into account possible changes in unit emissions or unit resource consumptions as a result of changes in technology or regulations, while a dynamic matrix  $C$  would allow for the consideration of changes in background environmental systems affecting impact mechanisms.

In order to assess the consequences of the decision, it is finally required to compare the results of the scenarios with and without the decision being analysed. The difference in generated impacts represents the broader environmental consequences related to the implementation of the new technology over the time frame considered.

LCA results are normally used for comparative assessments. In a traditional LCA the environmental impacts attributed to a product system represent the outcomes of the analysis, for subsequent comparisons to the environmental impacts attributed to other product systems (already studied or potentially object of future studies), which can be considered functionally equivalent. For example, the impacts of the technological system involved in the production of a biofuel can be compared to the impact of the technological system involved in the production of an equivalent amount of fossil-based traditional fuel, or another type of biofuel. The results are thus used to establish which is the best option from an environmental point of view and, assuming that nothing else will change in other systems (i.e. outside the system boundaries), it is deduced, for instance, how much would be the impact avoided through the production of one fuel with respect to the other. Instead, in this framework the focus is on the decision of implementing a biorefinery system, which also imply producing more biofuels: the effect of substituting a certain amount of alternative or traditional fuels is included by default among the effects originated from the initial decision. That is to say, the effects of the action on other product systems are valued on a par with effects across the product supply chain. The same reasoning applies to all products provided by the biorefinery system, which are assumed to substitute alternative or traditional products in the technosphere. In the proposed framework, the two groups of products (“new” and “old” products) are inherently compared modelling two situations: the “decision” scenario, in which the decision is taken, and a “zero-action” or “baseline”, in which the decision is not taken. Fig. 9 explains how the two types of comparison work differently: it can be said they correspond with the attributional and consequential concepts, elaborating on the representation provided by Weidema (2003) (see Fig. 2 - *The conceptual difference between attributional and consequential LCA* [40]). It should be noticed that comparison in consequential approach not necessary involves the assessment of global impacts, but it is usually focused solely on the portions of the global system which are expected to change due to a decision. However, here it is assumed that in principle any part of the global system is susceptible to change, since everything is in theory connected; input-output tables serve to mathematically represent this idea and trace possible changes in any part of the economic system.

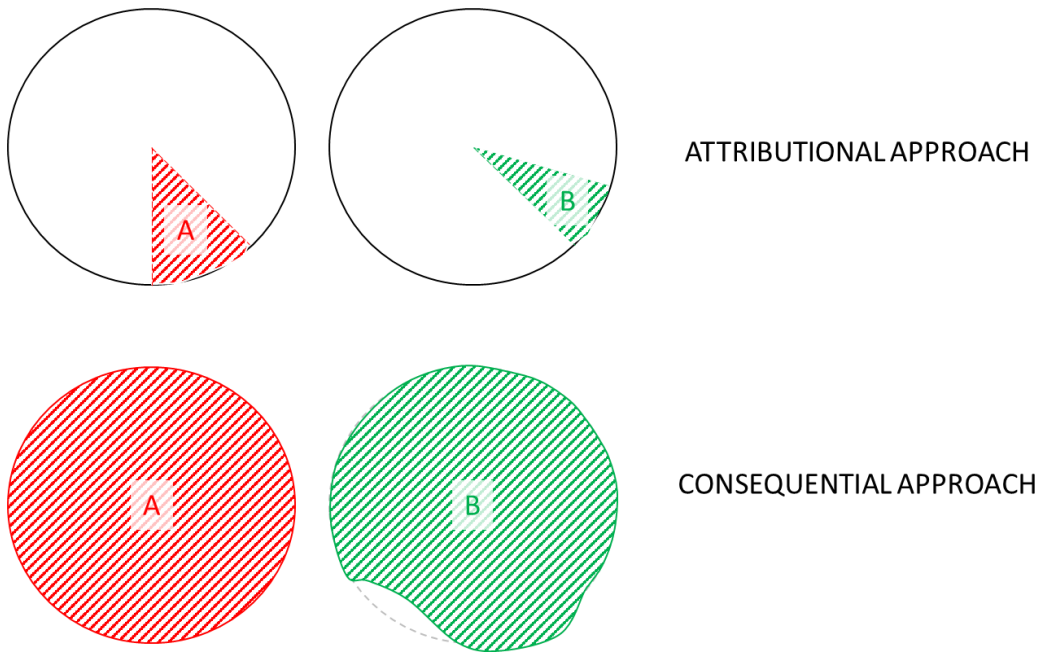


Fig. 9 – The conceptual difference of LCA comparison between the attributional and consequential approaches

The environmental consequences are the avoided or additional impacts due to the implementation of the technology, which can be simply derived by arithmetical difference between the results in the two situations considered, as in the following equation:

(Equation 15) 
$$\Delta h_t = h_{t,dec} - h_{t,no\ dec}$$

where the subscripts “dec” and “no dec” refer to the scenarios with and without the decision, respectively.

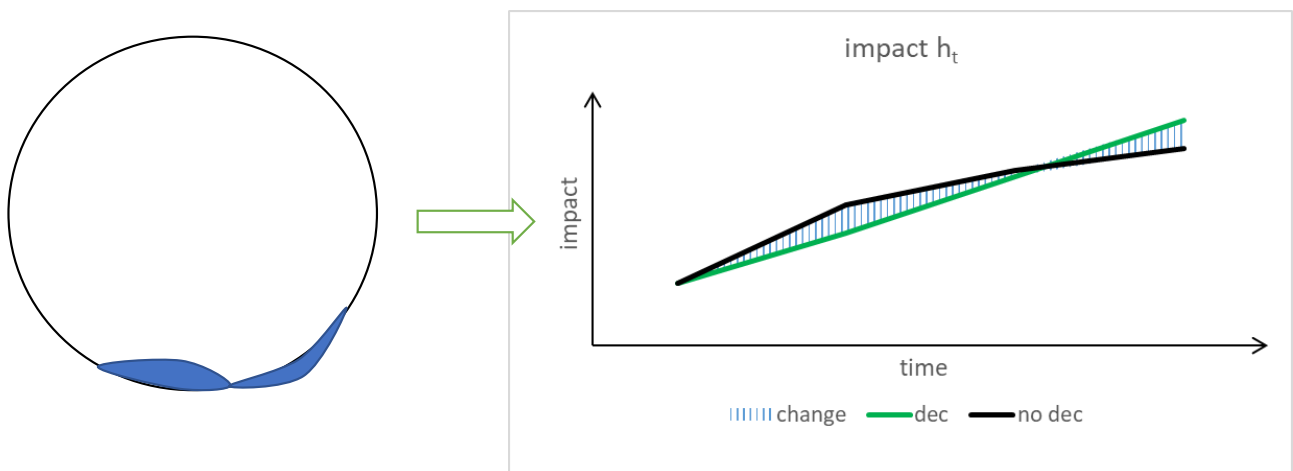


Fig. 10 – Dynamic representation of the impact according to the consequential approach

The cumulative change in impact can be simply calculated as the integral of the difference of the two functions over the time frame T considered:

$$(Equation 16) \quad \Delta \mathbf{h} = \int_0^T (\mathbf{h}_{t,dec} - \mathbf{h}_{t,no dec}) dt$$

In principle, the same reasoning applies to the sector total output  $\mathbf{x}$ , the change of which can be examined through the following equation:

$$(Equation 17) \quad \Delta \mathbf{x}_t = \mathbf{x}_{t,dec} - \mathbf{x}_{t,no dec}$$

# 5 Application to case study and results

## 5.1 Application of the framework to the case study

The framework, as presented in the previous chapter, was applied to the assessment of the following decision: “Building and running, in the European Union, biorefineries processing sewage sludge in the TCR-PSA-HDO combined process, up to 50 plants in 2030 processing 3 t/h of feedstock, and up to 300 plants in 2050 processing an average of 20 t/h”

### 5.1.1 Process-based data collection

The biorefinery system associated to the TCR-PSA-HDO technology was identified as a unique system providing multiple functions:

1. Gasoline production;
2. Diesel production;
3. Hydrogen production;
4. Electricity production;
5. Phosphorus production;
6. Sewage sludge management.

In Tab. 4, flows exchanged by the technology with other systems in the economy are presented. Flows corresponding to functions provided by the biorefinery system represent positive cash flows (underlined in the table), while other flows correspond to functions provided by other sectors of the economy to the biorefinery system and are to be intended as negative cash flows. Products related to functions provided by the system were labelled with “TSF” (from the name of the project, To-Syn-

Fuel) to be distinguished from other products in the economy. Prices were taken as far as possible coherent with the preliminary techno-economic assessment of the TSF project, which assumes prices of 577 EUR/t for diesel/gasoline equivalents, 75 EUR/MWh for power and 10 EUR/t as average feedstock gate fee (dry basis).

Tab. 4 – *Input and output flows of the foreground system in monetary terms (referred to 1 plant producing at 3 t/h for one year)*

<b>INPUTS</b>	<b>[EUR]</b>	<b>OUTPUTS</b>	<b>[EUR]</b>
<u>TSF Sewage Sludge</u>	1890000	<u>TSF Diesel</u>	392846
Tap water	3889	<u>TSF Gasoline</u>	248113
Softened water	23147	<u>TSF Electricity</u>	536336
Cooling water	333	<u>TSF Phosphorus</u>	2927342
Compressed air	127024	<u>TSF Hydrogen</u>	0
Natural gas	345601	Waste	43232
Nitrogen	166165	Process water	3781
NaOH	1147876		
H2SO4	188692		
Lubricating oil	1468		
HCl	89180		
Catalysts	1433085		
Steam	5444		
Concrete	3600		
Aluminium	116		
Copper	1036		
Steel	900		

With respect to the system analysed in the conventional LCA (Tab. 2), the same flows have been considered and, in addition, the main materials (concrete, aluminium, copper, steel) used for the building of the plant: specific data were not available, therefore data of a similar type of plant were used and adapted (ecoinvent process: “synthetic gas plant/p/CH/I”), allocating the flows over the operational lifetime of the plant (20 years) to simplify the analysis; indeed, working on the temporal resolution of the life cycle of the technology (e.g. considering the different timing of construction, use and dismantling phases) is out of the scope of this analysis.



### 5.1.2 Input-output data collection

EXIOBASE 3 [92] was chosen as reference database for this study, due to its high sectorial and regional detail. The EXIOBASE monetary IOTs cover the period from 1995 to 2011 and include 49 regions, precisely 44 countries (28 EU member plus 16 major economies) and 5 rest of the world regions (remaining countries in Europe, Asia, Africa, America and Middle East). However, only tables referred to 2011, considered the most representative year, were used to obtain the reference technical coefficients matrix, while the time series were used only to build projections for the demand vector (see section 5.1.4). Two versions of EXIOBASE 3 are available: product-by-product and industry-by-industry, which are compiled following two different approaches (more details can be found in *Eurostat (2008)* [96]). Product-by-product tables are used herein: they are based on the assumption that each product has its own typical input structure (product technology assumption), and classify all sectors through 200 products.

The IOTs by EXIOBASE 3 result in a large amount of data (about 800 MB compressed for each year), due to the high level of detail. For the purposes of the study, the IOTs were aggregated into 2 regions, Europe (EU-28) and Rest of the World (RoW), and 38 products. The regions' choice was dictated by the need to distinguish a region where a new technology can be implemented from a region where the same technology is not included. The products, instead, were chosen considering the best level of detail to associate correctly the flows identified in the foreground system analysis, whereas the rest of them were aggregated following their ISIC classification (International Standard Industrial Classification of all economic activities [97]). Also electricity products were left unaggregated, with the purpose to distinguish them when creating future electricity scenarios. Operationally, the Python module “pymrio” (Stadler, 2015) was employed to handle data and perform the aggregation of the original “200 products  $\times$  49 regions” IOTs into the new “38 products  $\times$  2 regions” IOTs. The correspondence files and the Python code used for the aggregation can be found in the Supplementary Material.

### 5.1.3 Hybridisation

The IOTs representing the world economy was thus completed with the inclusion of the new sector (augmentation), represented by the new products, “new” in the sense that they have their own specific input structure (according to the product technology assumption), different from other products

already present in the economy. Process data were used to simulate the physical input requirements of the new sector.

The augmentation regarded only region EU-28, assuming that the technology will be implemented exclusively in Europe. Therefore, the “38 products × 2 regions” IOTs were modified to include 6 additional products in region EU-28. The final tables resulted having 82 products (44 in EU-28, 36 in RoW) for the two regions.

It was assumed that the new products are going to substitute the products in the economy as presented in Tab. 5.

Tab. 5 – Assumption of substitution between new products and other products in the economy

<b>new products</b>	<b>substituted products</b>
TSF Sewage Sludge	EU-28 Inert Waste Incineration (30%) EU-28 Sewage sludge Land Application (50%) EU-28 Inert Waste Landfill (20%)
TSF Gasoline	EU-28 Motor Gasoline
TSF Diesel	EU-28 Diesel Oil
TSF Hydrogen	EU-28 Chemicals
TSF Electricity	EU-28 Electricity (Gas)
TSF Phosphorus	EU-28 P fertilisers, RoW P fertilisers

All energy products generated by TSF plants are expected to be sold in the domestic market within the European Union, for this reason the substitution involves only EU-28 products. Consequently, it was assumed that gasoline and diesel produced by the biorefinery will reduce the production of the fossil counterparts in EU-28 region.

Hydrogen is regarded as a chemical product, and it is an example of a specific product which is difficult to find in available IOTs and, in theory, the aggregated sector of chemicals should be chosen as substituted product; however, in this specific case the hydrogen flow was considered null, therefore this choice would not change the results. For what concerns electricity produced by the TSF system, it was assumed that the substitution will involve only the electricity production by the marginal unconstrained plants, likely gas power plants in a future perspective concerning Europe [58] [59];

this choice responds to a consequential approach, in which marginal data should be used whenever possible.

The function of sewage sludge management provided by the biorefinery was assumed to substitute other 3 management options, on the basis of their actual diffusion in Europe: recent data shows that sewage sludge in Europe is used mainly for land application, while the residual part is incinerated or landfilled [56] [57].

On the contrary, TSF Phosphorus, both for the quantities generated and for the typology of product, is likely to be sold also abroad substituting P fertilisers' products: it was assumed that the quantities exceeding the production levels corresponding to the 2030 target will be sold in the RoW region. Even possible variations for the products which are expected to be substituted can be addressed by means of a dynamic analysis, which is the next step of development for this framework.

The correspondences between intermediate flows identified for the foreground system and product categories in the IOTs, on which the compilation of new rows is based, are reported in Tab. 6.

Tab. 6 – *Product correspondences between the LCA system and the IO system*

<b>LCA product</b>	<b>IO product category</b>
Tap water	Collected and purified water, distribution services of water
Softened water	Collected and purified water, distribution services of water
Cooling water	Collected and purified water, distribution services of water
Compressed air	Electricity by gas
Natural gas	Natural gas and services related to natural gas extraction, excluding surveying
Nitrogen	Chemicals nec
NaOH	Chemicals nec
H2SO4	Chemicals nec
Lubricating oil	Lubricants
HCl	Chemicals nec
Catalysts	Chemicals nec
Steam	Steam and hot water supply services
Concrete	Cement, lime and plaster
Aluminium	Aluminium and aluminium products
Copper	Copper products
Steel	Basic iron and steel and of ferro-alloys and first products thereof
Waste	Inert Waste Landfill
Process water	Waste Water Treatment

It was assumed that, since the biorefineries are located in EU-28, the intermediate flows are all produced or managed in the same region. However, in principle, a mix of the two regions can be considered or regional changes over time can be modelled through the dynamic analysis. For

example, when the technology is implemented at larger scale, it is likely that markets other than the European one are involved by the higher demand of certain products used in the TSF technology.

It is clear that moving to an IO framework involves an increased level of aggregation. The use of EXIOBASE partially reduces this problem, providing one of the most detailed IOTs available. However, for some product typologies a rough aggregation in a wide-spectrum of product categories is needed, as can be seen for products which fall under the classification of chemicals. Another assumption involved the flow of compressed air, which was more conveniently converted into an equivalent amount of electricity to obtain that flow with the requested pressure; then, the input of electricity was assigned to electricity production by gas, to be consistent with the assumption of marginal technology considered for the electricity substituted by the new sector.

Finally, matrix **B** of environmental stressors was completed with the new products and their associated environmental flows. It can be seen that, in this case, the association between elementary flows and environmental extensions is not problematic, since the emissions at hand are well represented in the IO categorisation.

Tab. 7 – *Correspondences between the LCA elementary flows and the IO environmental extensions*

<b>LCA elementary flow</b>	<b>IO environmental extension</b>
CO <sub>2</sub> emissions	CO2 - combustion
N <sub>2</sub> O emissions	N2O - combustion
NO <sub>x</sub> emissions	NOx - combustion

#### 5.1.4 Inclusion of dynamic components

The IOTs obtained were then used to build an IO module, developed in a system dynamics environment. The open-source software Simantics System Dynamics (Version 1.35.0) [67], which is based on Java language and allows to handle array variables, was used for the modelling. Although the model itself is not causal, it was developed in this type of modelling environment to allow subsequent couplings with causal dynamic models that can generate the starting array coefficients (mainly for **A** and **y**, but also **B** and **C**); these models, however, are beyond the scope of the present work.

Matrix  $A$  was modified introducing time-dependent substitution factors  $sf(t)$ , which are calculated endogenously in the model:

$$\text{(Equation 18)} \quad sf_{S \rightarrow N}(t) = \frac{x_N(t)}{x_S(t)}$$

The numerator is the total output of the new product, which is a predicted value, coherent with the target for time  $t$  (obtained by Tab. 3, considering 20 t/h as average production capacity for the 2050 target). The denominator is the calculated value of total output of the substituted product at time  $t$ .

Since the IOTs used in the study refer to year 2011, they are not adequate to describe economic scenarios related to the following decades. For this reason, they need to be updated assuming certain trends occurring in the sectors of the economy, which can be expressed modifying technical coefficients in matrix  $A$  for modelling structural changes, and elements in vector  $y$  for modelling changes in final demand of each sector.

For all sectors except the electricity ones, future final demand was modelled based on historical trends, using the values from 1995 to 2011 contained in final demand vectors  $y$  of EXIOBASE, and performing a linear regression.

Technical coefficients in matrix  $A$  were modified specifically for electricity sectors, in order to reflect the future electricity mix outlined by future scenarios in the “World Energy Outlook” by the International Energy Agency (IEA) [98]. Data in the IEA report were aggregated to fit into the two regions of the model, and two different scenarios were considered: Current Policy Scenario (CPS) and Sustainable Development Scenario (SDS) (see Fig. 11). Coefficients in matrix  $A$  were thus increased or decreased by factors that reflect the change in the energy mix from year to year. The same scenarios by IEA were used to modify the final demand for electricity sector in vector  $y$ .

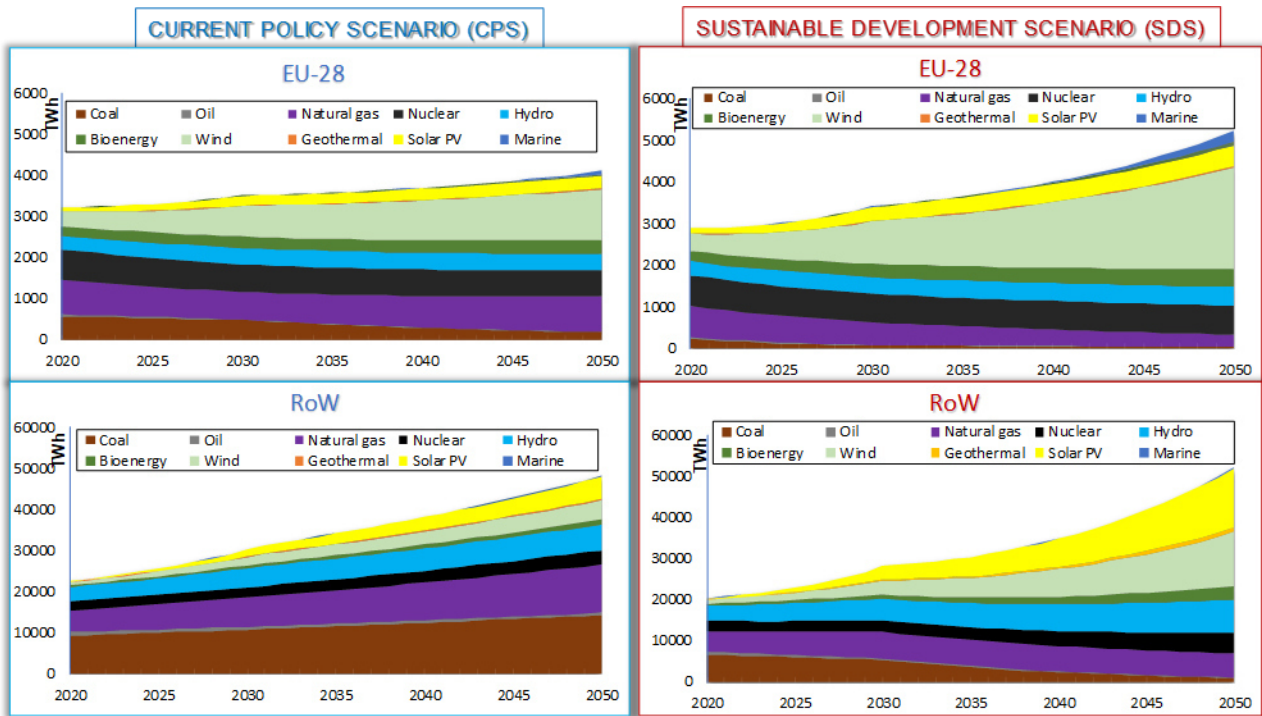


Fig. 11 – *Electricity scenarios used in the model*

### 5.1.5 Impact assessment

The following impact categories were considered in this study:

- global warming, 100 years (GWP);
- photochemical oxidation (POCP);
- acidification (AP);
- eutrophication (EP);
- human toxicity (HTP).

For the characterisation step, the CML 2001 impact assessment method [57] was followed.

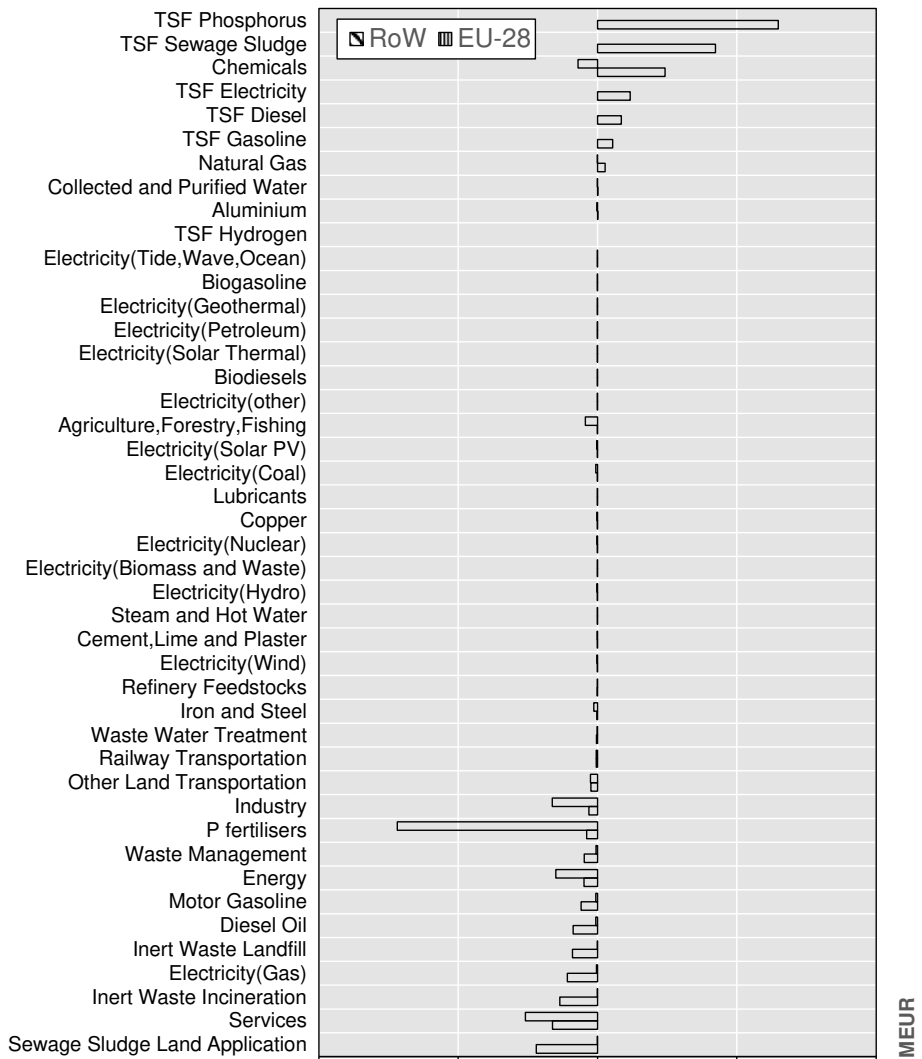
The matrix  $C$  of characterisation factors was retrieved by the CREEA project [99] and is provided in the SM (8.3).

The two main scenarios for this specific case study will be indicated as “TSF” and “noTSF” from hereafter. For convenience, in cases where  $\Delta h_t$  assumes negative values, its sign is changed to positive and it is referred as “impact savings”, which means that the “TSF” scenario is characterized by lower impacts than the “noTSF” scenario.

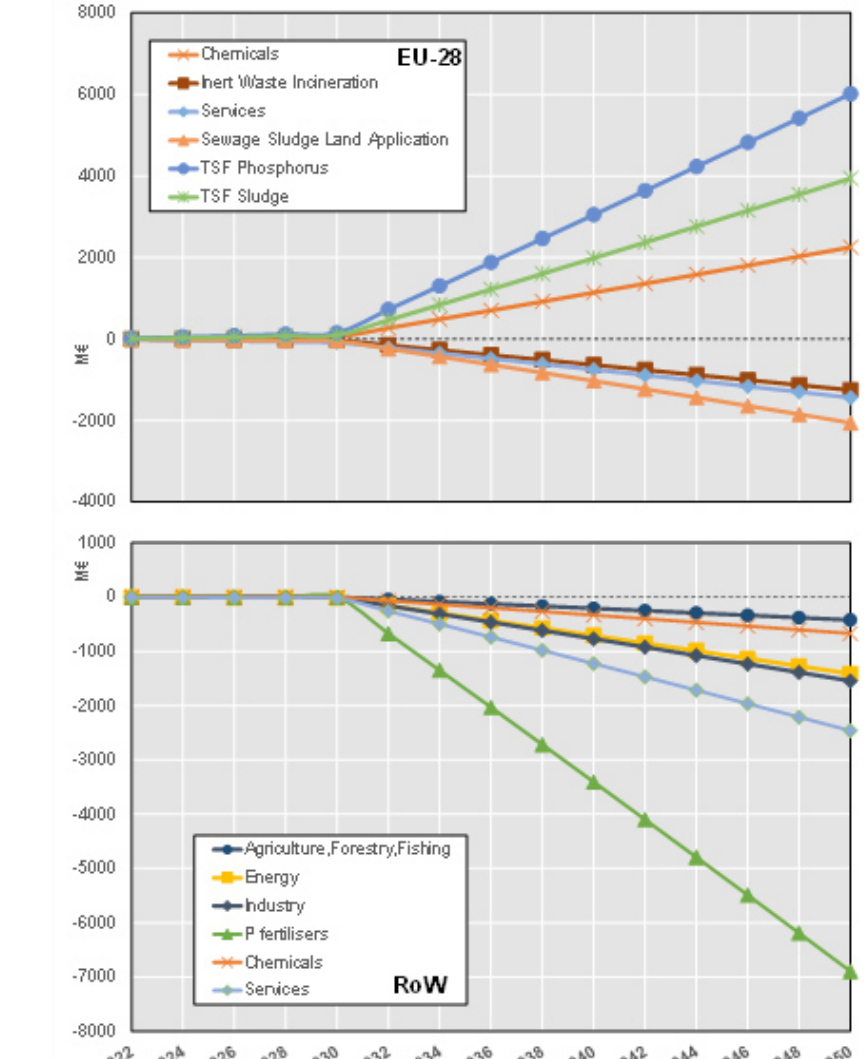
## 5.2 Results

### 5.2.1 Sector total outputs

In the model, the vector  $\mathbf{x}$  of sector total outputs was calculated for each time step with (Equation 13). The comparative assessment consists in the arithmetical difference between vector  $\mathbf{x}$  in “TSF” and “noTSF” scenarios. In a first step analysis, it is useful to examine the difference in vector  $\mathbf{x}$ , in order to understand which sectors are mostly affected by the introduction of the TSF technology, regardless of the environmental impacts.



A)



B)

Fig. 12 – Change (2022-2050) in sector total outputs in the CPS scenario. A) Cumulative change. B) Time trends of change for selected sectors.



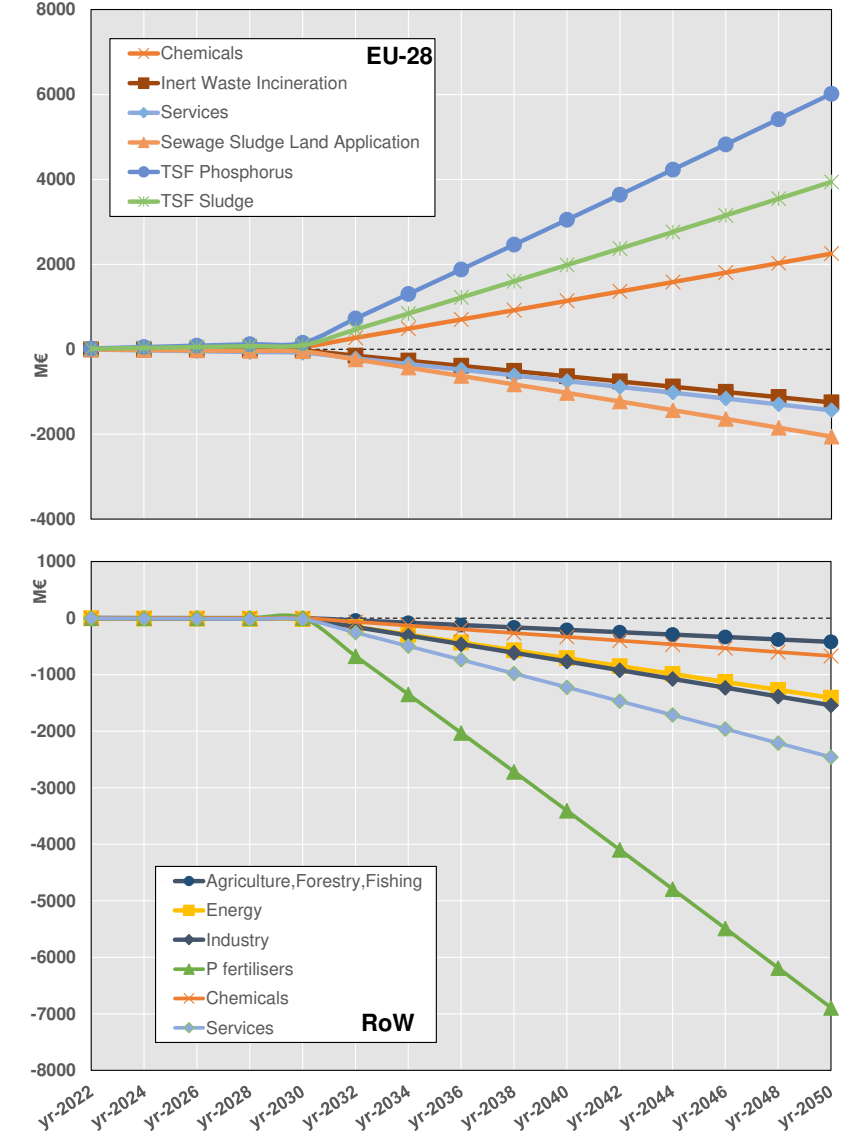
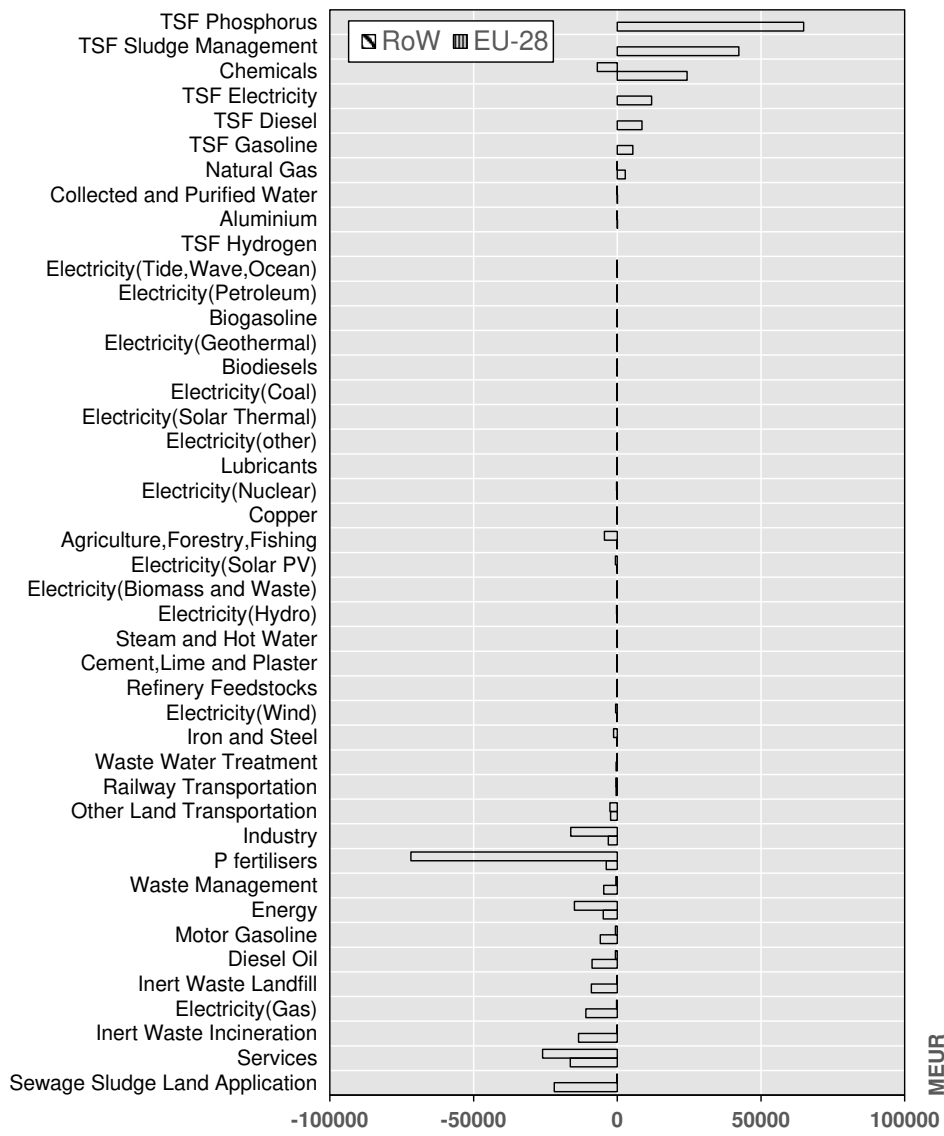


Fig. 13 – Change (2022-2050) in sector total outputs in the SDS scenario. A) Cumulative change. B) Time trends of change for selected sectors.

Fig. 12 shows the change  $\Delta x$  in sector total outputs in CPS scenario; the left part of the figure outlines the total change cumulated in each sector of the economy for the whole period 2022-2050; the right part of the figure shows the time trends of change for the most affected sectors in the two regions. Obviously, products associated with the TSF technology exhibit a growth in production, as imposed by the model. The most affected sectors are clearly related to products substituted by the new ones, such as sewage sludge for land application, inert waste to incineration, electricity by gas, inert waste to landfill, diesel oil and gasoline in the EU-28 region, and P-fertilisers both in EU-28 and RoW regions; all these products exhibit a decrease in their production. Other sectors are affected as well, being directly or indirectly linked to sectors that have changed their output. Among them, sectors which are particularly involved in providing products for the functioning of the TSF technology shows an increase in production, above all EU-28 chemicals. Apparently, electricity sectors other than production by gas are not significantly involved by the change. Sectors indirectly affected include services, energy and industry sectors, with negative changes in product outputs, in particular in RoW region.

For what concerns the time trends of change in total outputs, it can be seen that the most affected sectors show a linear increase, since the main driver is the linear growth of the TSF technology to reach the targets for 2030 and 2050 that has been modelled. The growth is definitely most significant from 2030 onwards, when the technology is expected to be mature for a further implementation on a larger scale.

Similar trends and values can be found for the SDS scenario, shown in Fig. 13. While apparently only small differences for the change  $\Delta x$  in sector total outputs are found between the two electricity scenarios, it is possible that significant differences can still be found for the change  $\Delta h$  in impacts, which is dependent also on the environmental stressors associated to each sector. The change  $\Delta h$  in impacts is investigated in the next section.

At this stage it is also possible to check whether the model reproduces the assumptions made for specific sectors. By way of example, the trend of  $x$  for the P fertilisers sector are shown with respect to the two situations being compared, “TSF” and “noTSF”, for the regions EU-28 and RoW, in Fig. 14 and Fig. 15 respectively. The trends are consistent with the assumption in section 5.1.3, according to which quantities of TSF Phosphorus exceeding 2030 production levels will be sold in the RoW region. Indeed, EU-28 P-fertilisers production faces a decrease (i.e.  $\Delta x$  has negative values) due to product substitution, which grows consistently up to 2030, and then remains approximately constant up to 2050. On the other hand, RoW P-fertilisers is not affected by a change up to 2030, when negative

values of  $\Delta x$  compare, with a growing trend. It can be observed that no relevant changes are present for this sector between the CPS and SDS scenarios, since both the absolute and relative values of  $x$  are not influenced by the electricity mix.

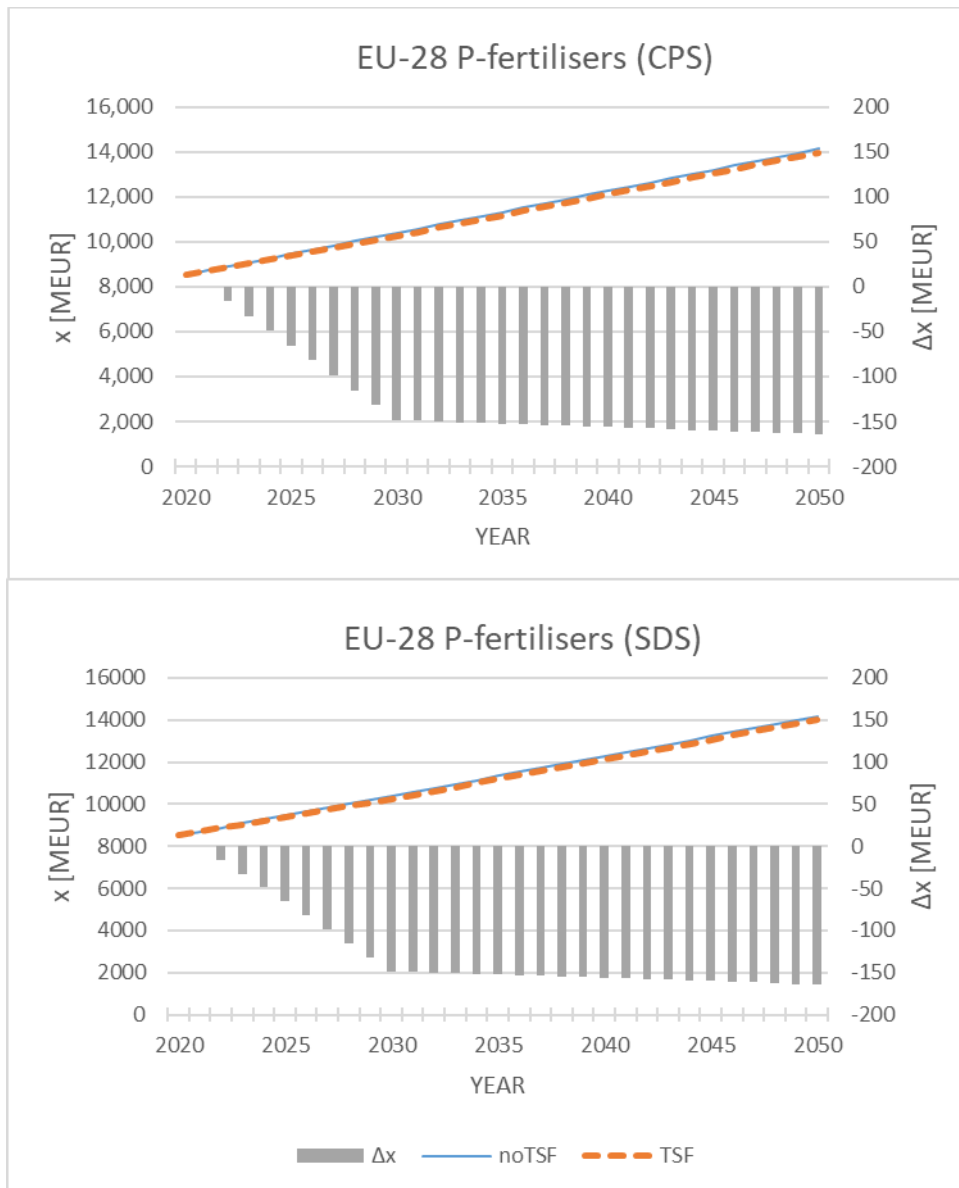


Fig. 14 – Sector total outputs (lines; left axis) and change in sector total outputs (bars; right axis) for P fertilisers sector in EU-28 in the CPS and SDS scenarios

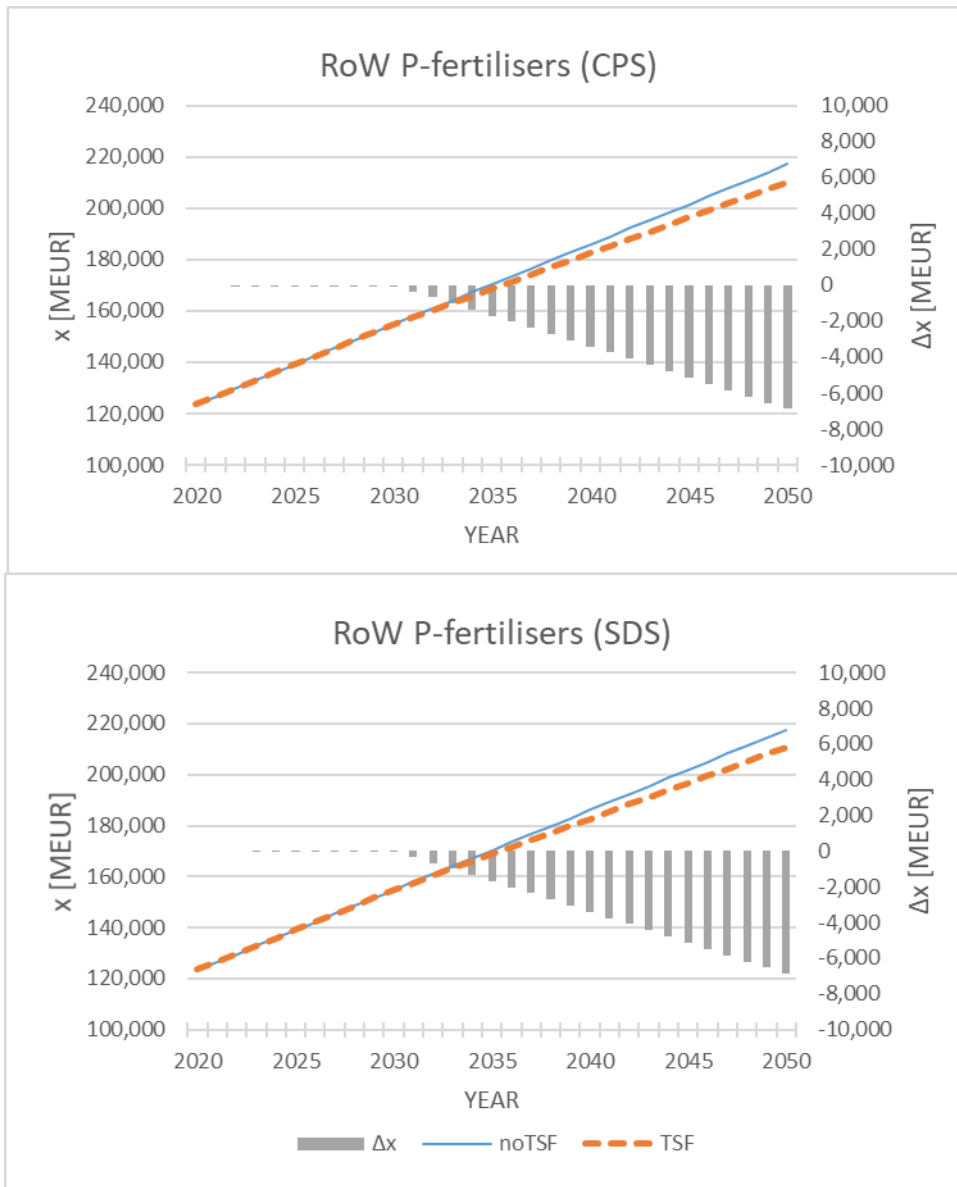


Fig. 15 – Sector total outputs (lines; left axis) and change in sector total outputs (bars; right axis) for P fertilisers sector in RoW in the CPS and SDS scenarios

On the contrary, sector total outputs in the sectors related to electricity production are expected to change consistently in the two scenarios. In particular, they are assumed to follow the energy share of the IEA scenarios. By way of example, absolute values of sector total outputs for Electricity in the RoW region and the TSF+SDS scenario are shown in Fig. 16. It was verified that the  $x$  values return the same energy shares of the SDS scenario by IEA data, as presented in Fig. 17.

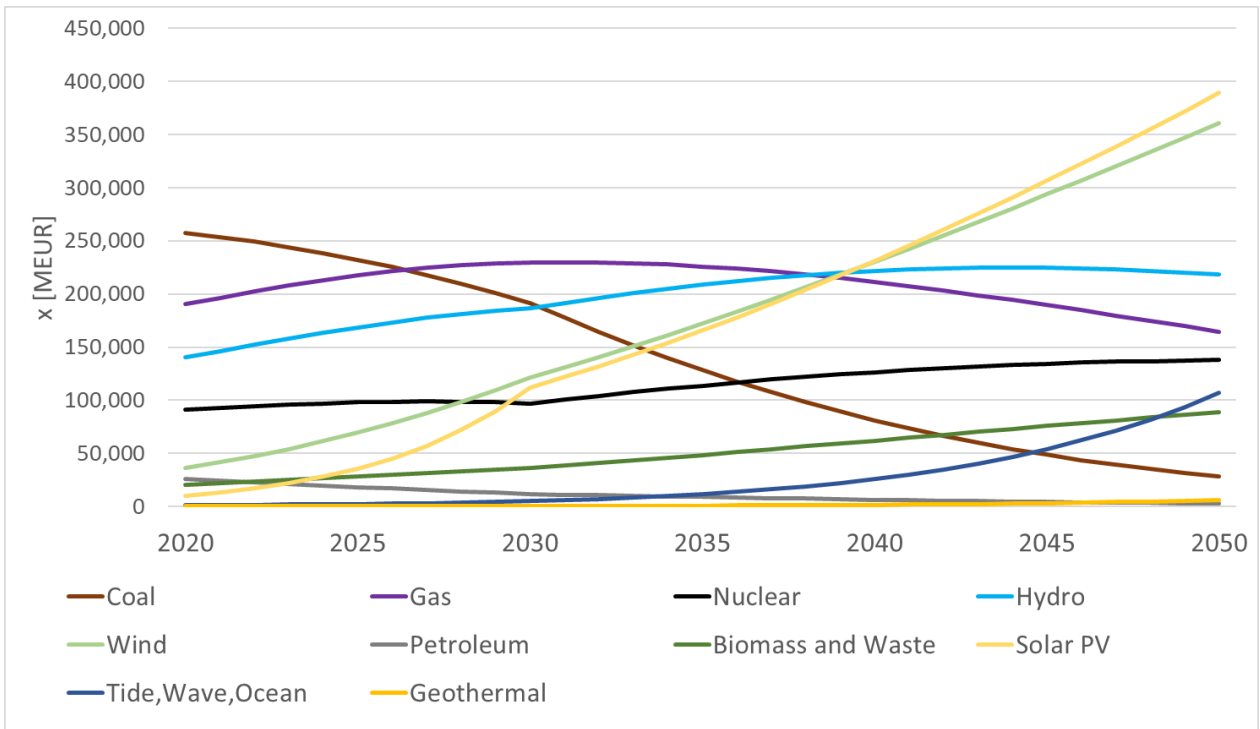


Fig. 16 – Sector total outputs of Electricity sector in RoW region (TSF, SDS scenario)

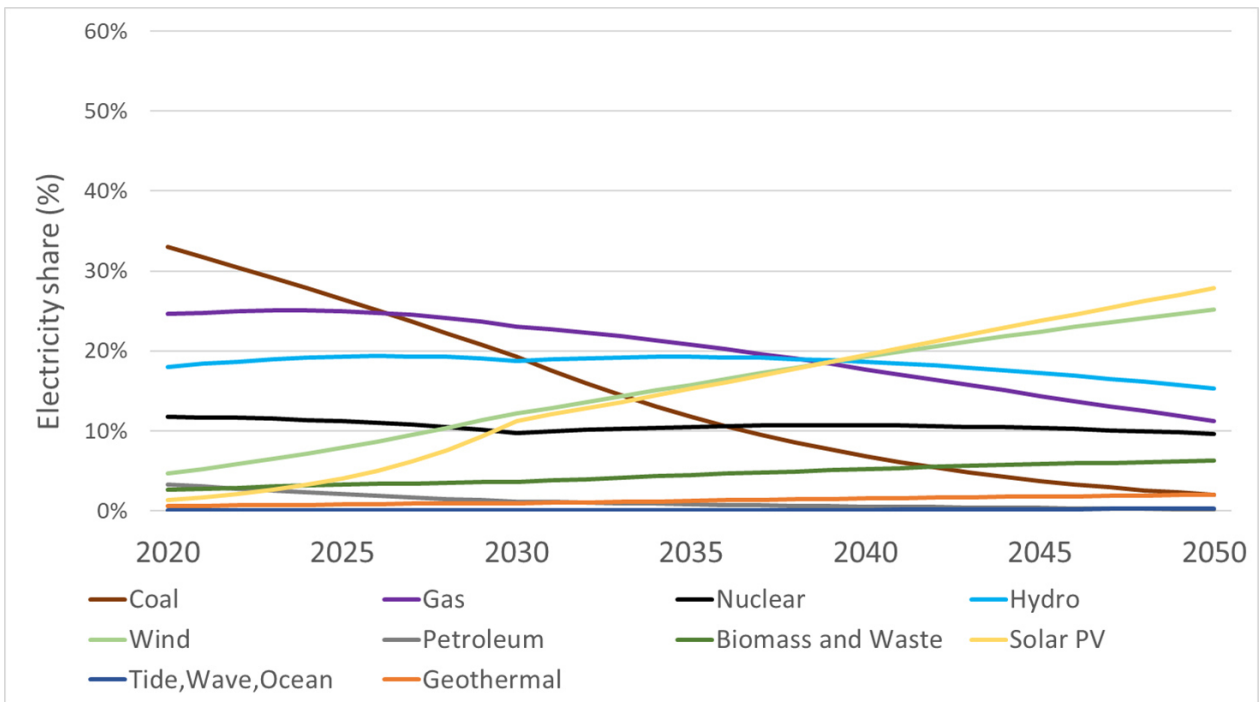


Fig. 17 – Energy shares according to the SDS scenario for RoW region

## 5.2.2 Impacts

The ultimate objective of the model is to measure the environmental consequences, in terms of change in impacts, which follow the decision at hand. Applying Equation 14 and Equation 16 in sequence, the total change in impacts can be obtained. For convenience, since  $\Delta h$  assumes mostly negative values, its opposite  $-\Delta h$  is shown and referred to as “impact savings” (or just “savings”): if positive values are presented for impact savings, it means that the “TSF” scenario is characterized by lower impacts than the “noTSF” scenario.

In Tab. 8 impact savings are shown for both electricity scenarios, and in Fig. 18 the two scenarios are compared reporting the values in percentages.

Tab. 8 – *Impact savings of the TSF technology*

impact	unit	Total savings		Savings per MEUR (2022-2050)		Savings per MEUR (annual average)			
		CPS	SDS	CPS	SDS	CPS	$\sigma$	SDS	$\sigma$
GWP	kg CO2 eq	1.27E+11	1.11E+11	1.91E+06	1.68E+06	8.70E+05	17%	7.78E+05	14%
POCP	kg C2H4 eq	3.17E+07	2.94E+07	2.39E+02	2.21E+02	2.10E+02	22%	1.96E+02	21%
AP	kg SO2 eq	6.53E+08	5.84E+08	4.91E+03	4.39E+03	4.14E+03	30%	3.74E+03	29%
EP	kg PO4--- eq	5.85E+07	5.56E+07	4.40E+02	4.18E+02	3.62E+02	34%	3.45E+02	34%
HTP	kg 1,4-DB eq	2.84E+11	2.83E+11	2.14E+06	2.12E+06	1.81E+06	29%	1.80E+06	29%

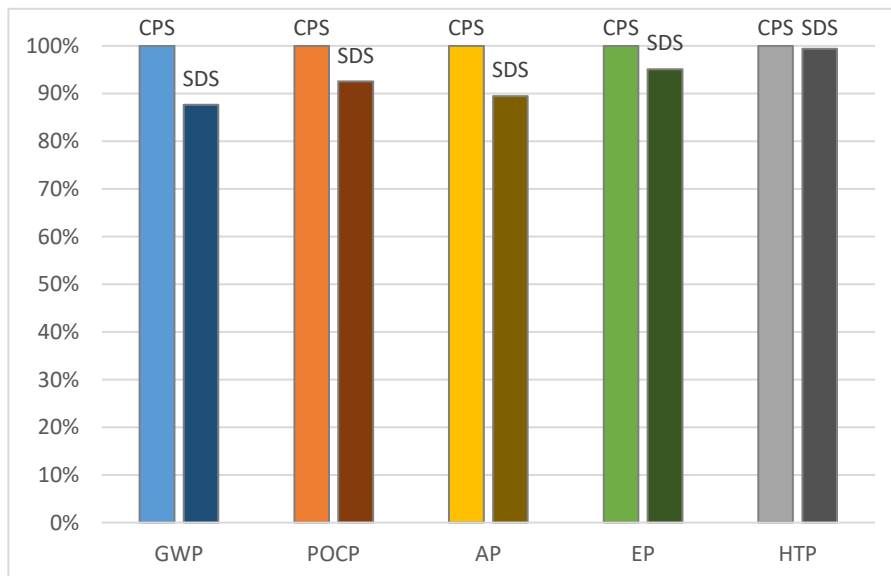


Fig. 18 – *Comparison (%) of impact savings of the TSF technology in the CPS and SDS scenarios*

When observing these results, it is evident that the impacts of the technology depend on the policy context. Specifically, impact savings associated to the implementation of the TSF technology appear to be lower in a context of more ambitious environmental policies, albeit to varying degrees depending on the impact category. This outcome can be explained considering that a more challenging (from an environmental point of view) technological benchmark results in a reduction of the environmental benefits of a potentially “green” technology. Precisely, the main difference between the two scenarios can be noted in the impacts of GWP (>10%) and AP (10%), while no relevant difference can be detected with regard to HTP impact.

Furthermore, observing Fig. 19 and Fig. 20, it can be noticed that, although the technology is implemented only in EU-28, a greater part of the environmental benefits is obtained in the RoW region. Indeed, the impacts avoided the EU-28 region represent a percentage of the total impact savings ranging from 2% in the EP impact category to a maximum of 14% in the GWP impact category, with no relevant differences between the CPS and SDS scenarios.

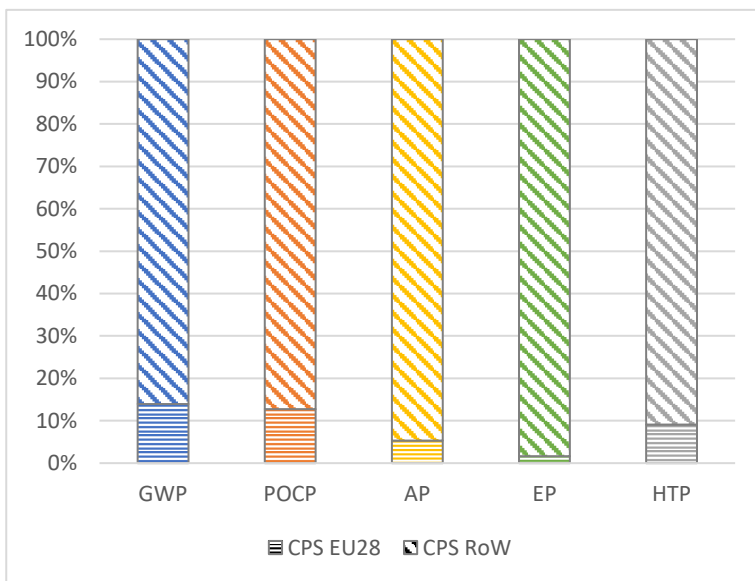


Fig. 19 – Contribution (%) of the EU-28 and RoW regions to the impact savings of the TSF technology (CPS scenario)

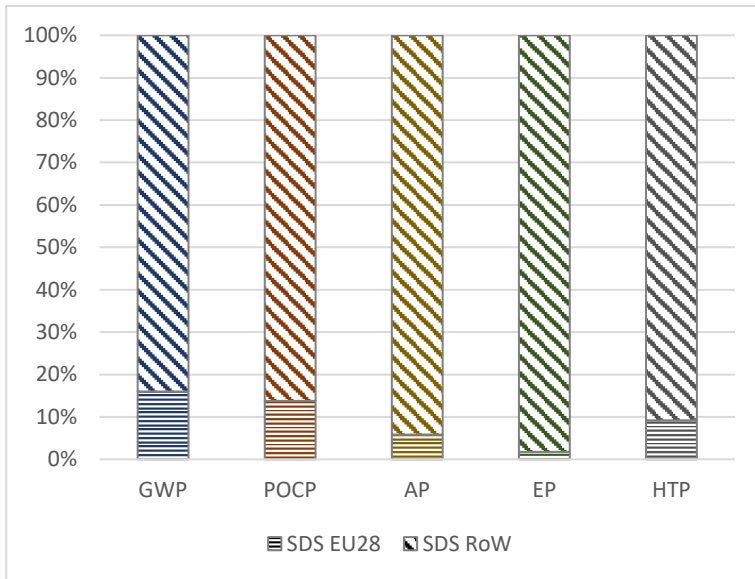


Fig. 20 – Contribution (%) of the EU-28 and RoW regions to the impact savings of the TSF technology (SDS scenario)

Tab. 8 also reports the impact savings per unit of economic revenues generated through the operation of the new sector. In this way, the impact savings due to TSF technology can be evaluated also in relation to the yearly relevance, in economic terms, of the decision analysed. Two types of impact savings per MEUR of TSF revenues are calculated and reported in the table. In the first place, the 2022-2050 values refer to the ratio between the total impact and the total revenues generated by the TSF plants over all the time span. Secondly, the annual average is obtained as average of the ratio between impacts and revenues calculated for each year of the time frame. The standard deviation of the latter provides a measure of the variability of the impact intensity that can be detected in such a dynamic analysis in which different parameters vary over time, affecting the environmental performance of the assessed technology. It can be seen that this variability spans from 14% to 34%, suggesting that a static analysis would not capture important differences over the time frame considered.

This variability can be observed more precisely in the figures reporting the time trends of impact savings per monetary unit. For instance, in Fig. 21 yearly impact savings are shown for the GWP impact category. The following information can be deduced by the trends observed in the figure:

- The main source of variability in both scenarios is determined by the gap between two groups of values (until 2030 and after 2030); this behaviour can be explained considering that, in accordance with assumptions, after 2030 the TSF technology directly affects also the “P fertilisers” sector in RoW, where highest GHG emissions are associated to the product unit with respect of the EU-28 counterpart. Consequently, the TSF technology is likely to increase its environmental



performance as it becomes more capable of affecting the RoW economy. This also suggests that a possible future implementation of this technology also outside European Union would be even more beneficial for the environment.

- There is a slight reduction of the GWP impact savings which occurs constantly over time; the reason can be attributed to an increase in the use of renewable energy, which progressively reduces the GWP of the technologies against which the bioenergy at hand is measured.
- Higher GWP impact savings can be obtained in the CPS scenario (light blue bars), and the gap against the SDS scenario (dark blue bars) exhibits a slight increase over time; also this effect can be attributed to the amount of renewable energy in the electricity mix and its lower GWP: this amount is not only always higher in the SDS scenario, but also increases faster than in the CPS scenario.

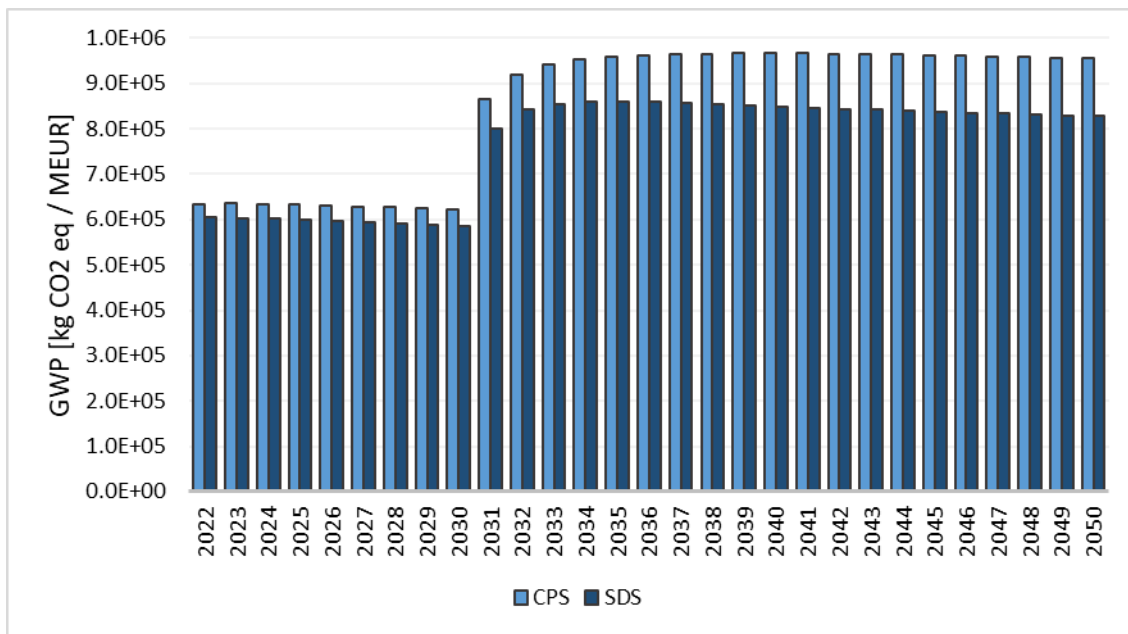


Fig. 21 – Yearly GWP impact savings per MEUR of revenues in the CPS and SDS scenarios

Similar figures for the other impact categories are obtained and shown in the following. However, some differences can be observed with respect of what was found for the GWP impact category. The effect of shifting to RoW P-fertilisers (as main substituted product for the new product TSF Phosphorus) proves to be beneficial for all impact categories: indeed, the impact savings of the production unit always exhibit a net increase when this shift takes place, and they tend to settle on constant values after 3-4 years, that is when the quantities of TSF Phosphorus sold in the RoW far exceed the quantities sold in EU-28. There is still a difference, but not large (even negligible for HTP), between the impact savings in the two electricity scenarios, which just confirms what was found in Fig. 18 about cumulated changes. Beside this, no other trends can be detected over time, or

at least they are less evident than in the case of GWP impact. This fact suggests that the change in the electricity mix have a significant influence on the GWP impact, whereas other impacts are not particularly affected. This does not mean that the analysis of technology in a dynamic context is not important for impacts other than GWP, but that other situations would need to be modeled over time in addition to the variation of the energy mix to understand how also these impacts could potentially vary in a changing context.

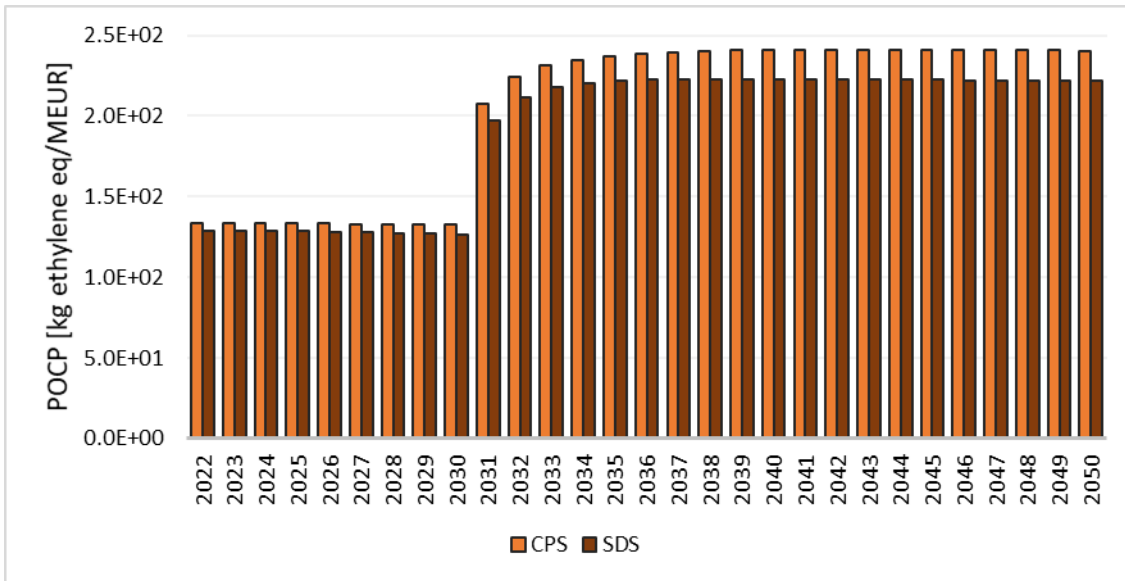


Fig. 22 – Yearly POCP impact savings per MEUR of revenues in the CPS and SDS scenarios

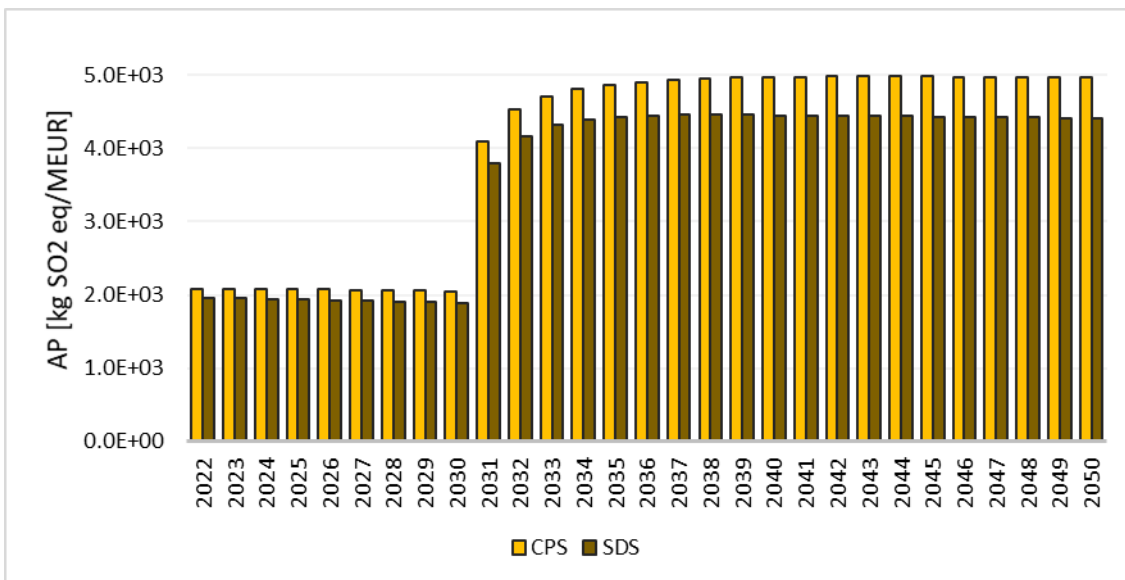


Fig. 23 – Yearly AP impact savings per MEUR of revenues in the CPS and SDS scenarios

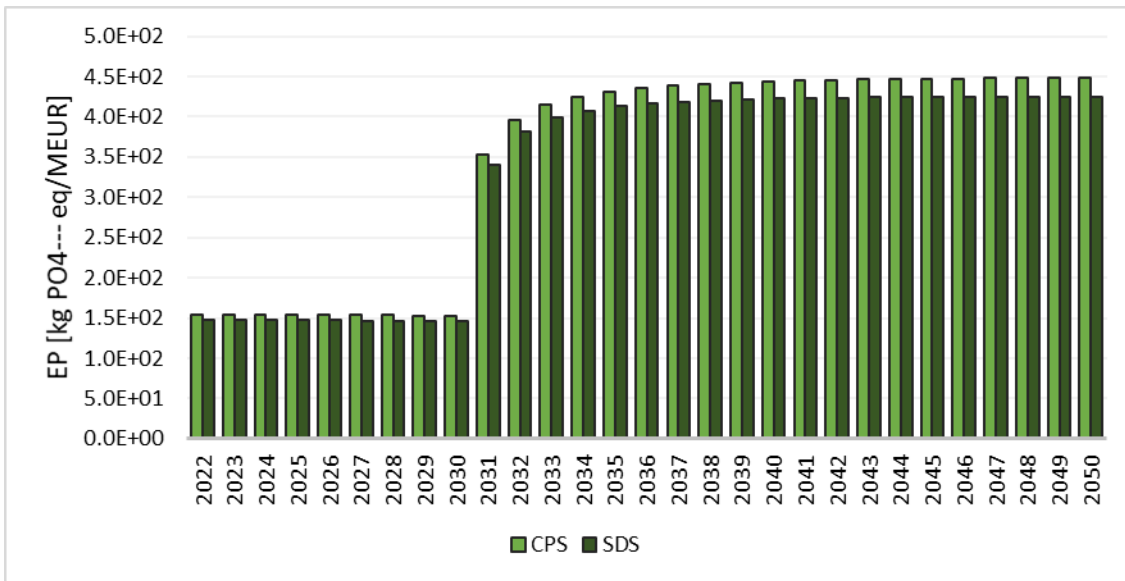


Fig. 24 – Yearly EP impact savings per MEUR of revenues in the CPS and SDS scenarios

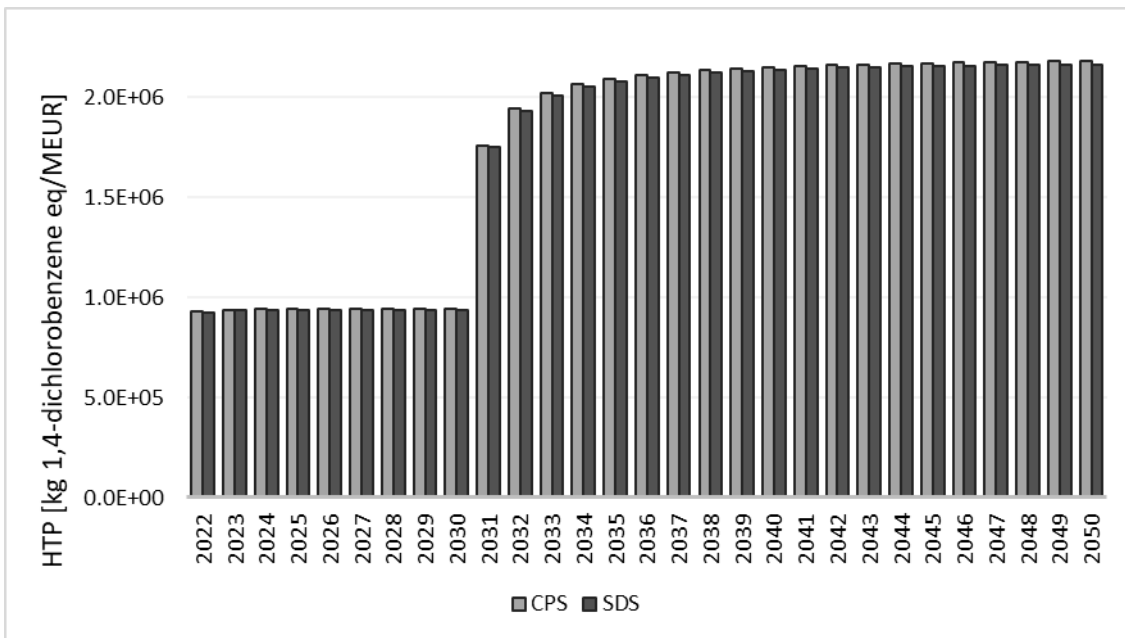


Fig. 25 - Yearly HTP impact savings per MEUR of revenues in the CPS and SDS scenarios

Similarly to what was done for sector total outputs, also the change  $\Delta h$  in impacts can be analysed differentiating the contributions by sector. In Fig. 26 it can be seen which are, among the affected sectors, the most contributing to the GWP impact change. The graph confirms that the environmental benefits of the TSF technology would mainly come from the substitution of P fertilisers produced in RoW, and secondly from the substitution of electricity produced by gas in EU-28. Interestingly, an important contribution also comes from other sectors in RoW only indirectly affected, especially the “Energy” sector, which includes different typologies of energy-related products (see SM 8.1).

On the other hand, the implementation of the TSF technology will require the production of additional chemicals, used in the TCR/PSA/HDO process, and natural gas to meet the additional demand of thermal energy for the drying of sewage sludge in the pre-treatment phase. Therefore, the analysis suggests that further improvements in the GWP performance can be obtained implementing solution for reducing the use of chemical products and for performing the drying of biomass with the only contribution of renewable sources.

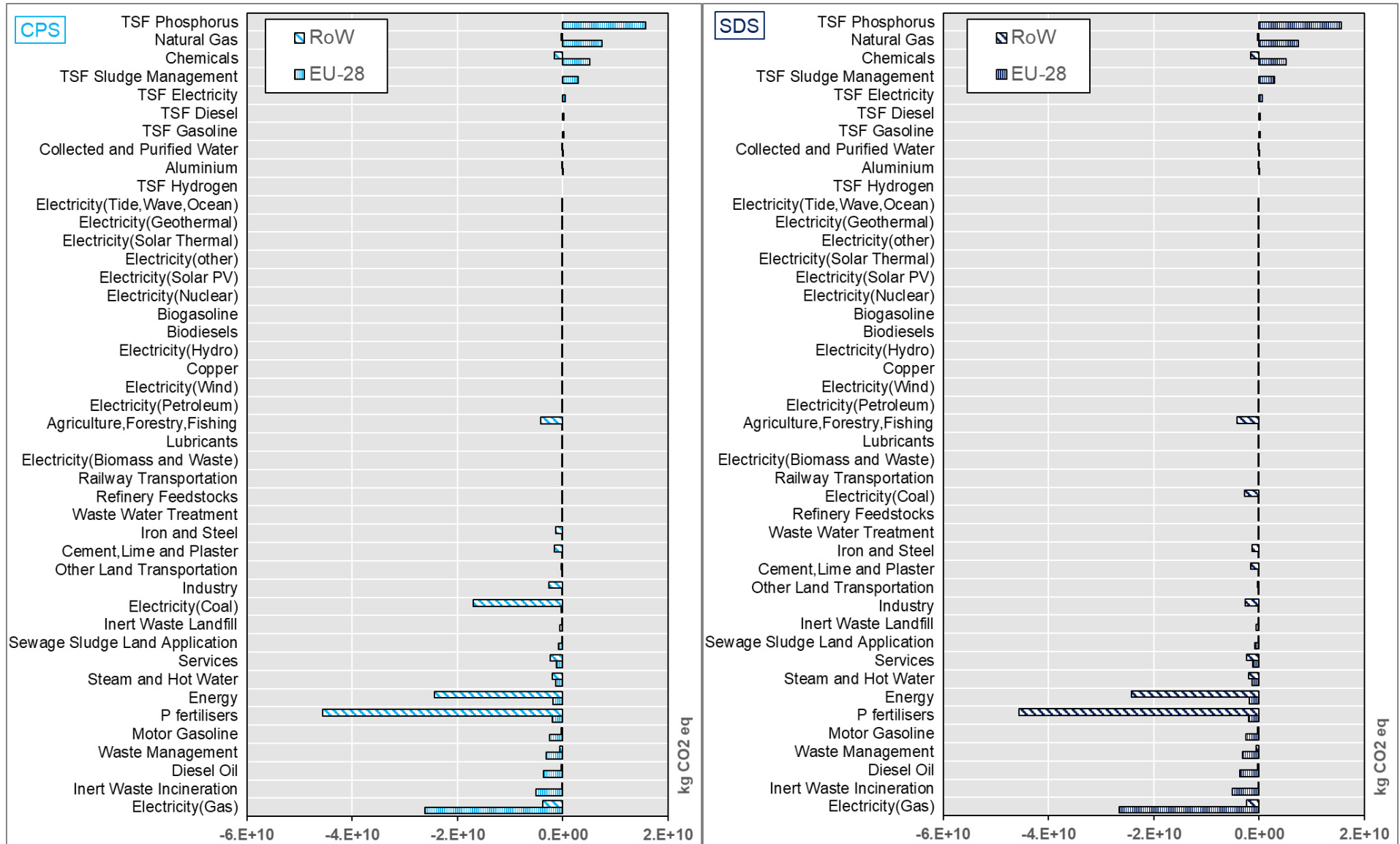


Fig. 26 – GWP impact by sector of the TSF technology

Furthermore, it can be noticed that the main difference between the two scenarios concerns the contribution of electricity by coal in RoW, which is considerably reduced in the SDS scenario. The explanation can be sought for looking at the time trends for this specific sector. Fig. 27 and Fig. 28 show the trends for the GWP impact of the “Electricity(Coal)” sector, in EU-28 and RoW respectively.

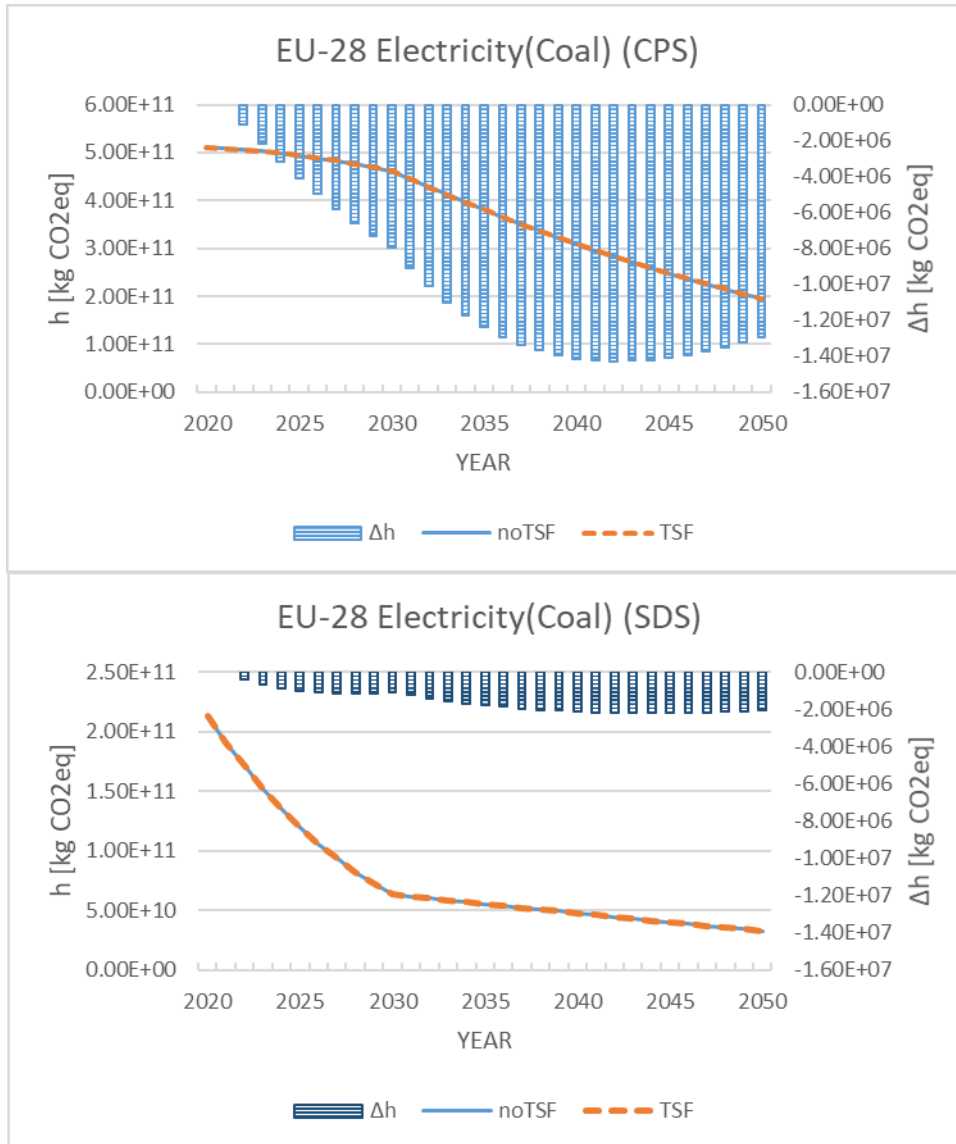


Fig. 27 – GWP impact (lines; left axis) and change in GWP impact (bars; right axis) for Electricity(Coal) sector in EU-28 in the CPS and SDS scenarios

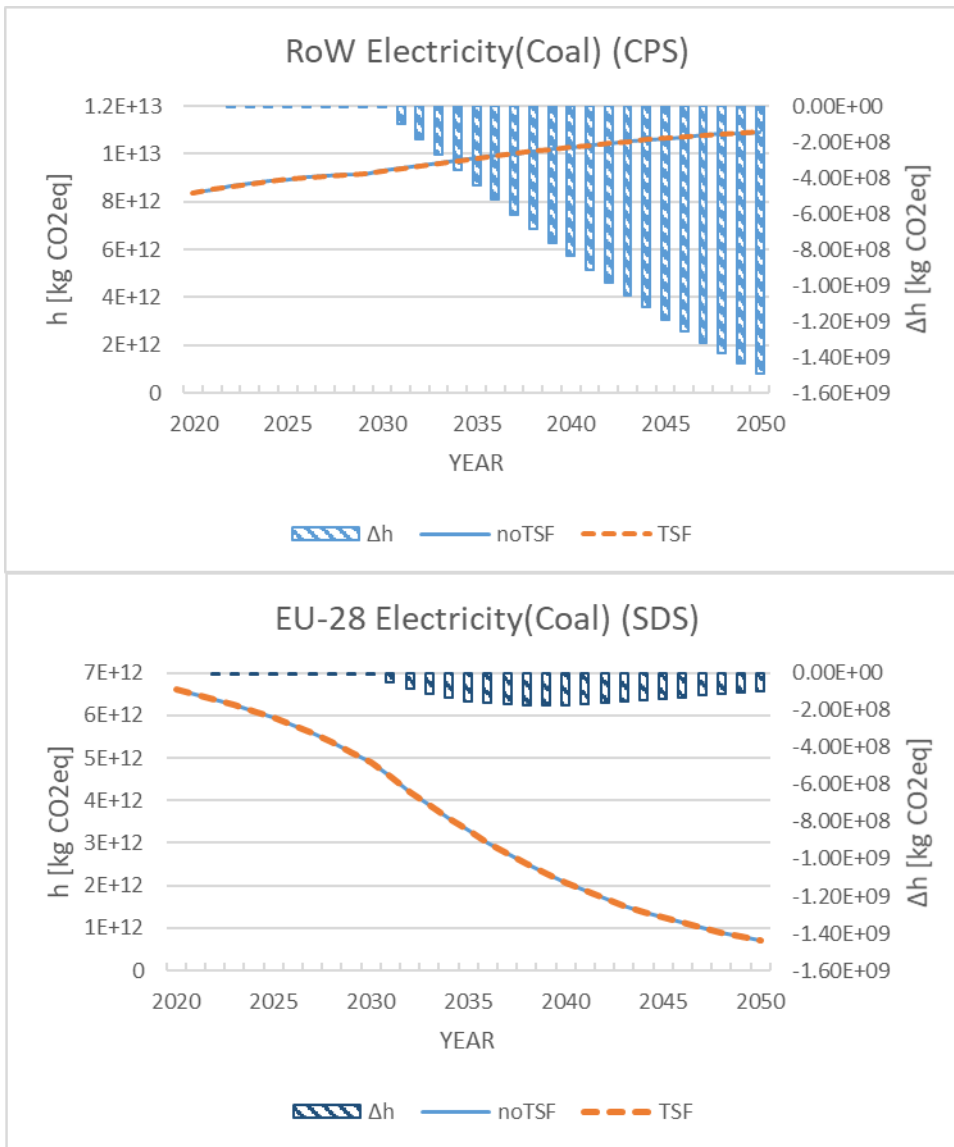


Fig. 28 – GWP impact (lines; left axis) and change in GWP impact (bars; right axis) for Electricity(Coal) sector in RoW in the CPS and SDS scenarios

First of all, it can be noticed that in the SDS, in both regions, the GHG savings ( $\Delta h$ ) related to this sector are always small compared to the CPS scenario. The reason can be found observing the time trend in absolute values of the impacts in the two scenarios: in a context of decreasing absolute impacts, due to phase out of coal industry, the capacity of the new technology to obtain GHG savings avoiding electricity production from coal is reduced. This effect can also be seen in the last part of the time frame (2042-2050) for CPS in EU-28, when the growth trend of yearly GHG saving is reversed. This is reasonably what could be expected in the future, when the lesser presence of fossil sources would reduce the possibility for “green” technologies to avoid their use, and together would increase the competition among “green” technologies themselves. One last thing can be observed from these figures: the sector in RoW region, contrarily to the one in EU-28 region, starts being

consistently affected only after 2030; this is an indication of the interlinkage between this sector and that of P fertilisers in the RoW, which is directly affected only starting from 2030 (confirmation of this can be found in the *A* matrix). This result confirms the importance of assessing the environmental impact of a given technology both in the context of different possible future global scenarios and with extended boundaries. Indeed, the sector “Electricity(Coal)” proved to be potentially relevant for the results, being an indirectly affected sector, and at the same time its relevance is strictly scenario-dependent. These aspects cannot be captured, for instance, in a conventional LCA in which a black-box LCA database for the process of P-fertilisers production is included in the model (when applying substitution, to account for the phosphorus co-product). In the best case, a dynamic perspective would involve the dynamic change in the directly substituted products and direct requirements of the foreground system; in the event that major contributions to impacts lie in far upstream inputs, they would be not addressed by any dynamic consideration.



# 6 Discussion

## 6.1 Insights for the case study

Differently from a typical product LCA, this research aims at quantifying the potential environmental consequences of a decision, rather than attributing an environmental performance to a product and its related function. For this reason, the outcomes of the model are not used for comparison purposes with other product systems, but they provide a quantification of the expected environmental consequences of a decision, which can be evaluated comparing the magnitude of the environmental outcomes with respect of the targets of the current environmental policies.

In this case, the decision to implement the biorefinery system associated with the TCR-PSA-HDO technology, in the EU and at the given scale up to 2050, can be eventually confronted with European targets. Environmental policies and targets tend to focus on climate change issues; for this reason, the more relevant analysis can be done in the context of GHG reduction targets.

Specifically, EU is committed to reduce its GHG emissions by 55% in 2030 with respect to 1990 emission levels, according to the most updated “2030 Climate Target Plan” [100]. This closer target have been fixed in the context of a highly ambitious pathway to climate neutrality by 2050, according to its long-term strategic vision [101].

Considering the current levels of GHG emissions, it would require an average reduction of 146 Mt CO<sub>2</sub>eq per year to meet the 2030 target and of 128 Mt CO<sub>2</sub>eq per year to meet the 2050 target. It means that year by year, an increasing quantity of yearly GHG savings is required, to be found in technological innovation, reduced consumption, or improved efficiency. This study shows that TSF technology is capable of saving from 111 to 127 Mt CO<sub>2</sub>eq up to 2050 (see Tab. 8), reaching a top contribution of 0.23 ÷ 0.26 % in 2050 to the EU reduction target. Fig. 29 shows how this contribution would rise over time, obtained from confronting yearly GWP savings by the technology with yearly GHG emissions reduction to reach the EU targets.

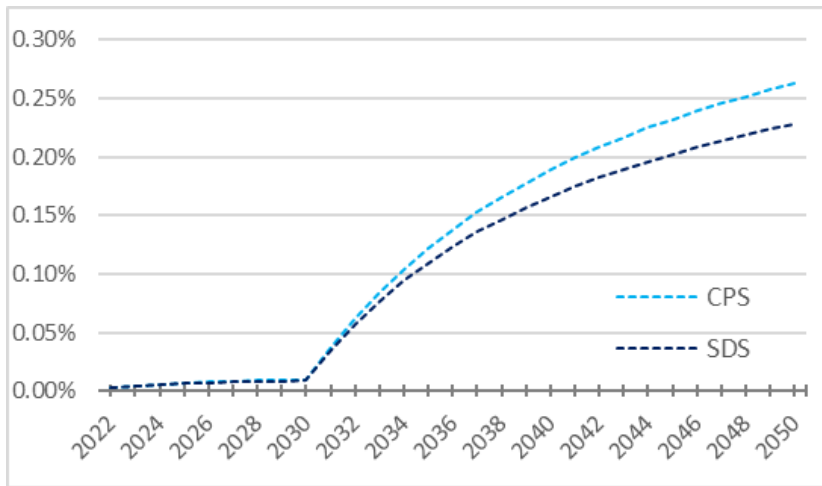


Fig. 29 - Yearly contribution (%) of TSF technology to targets of GHG emission reduction of EU in the period 2022-2050

This contribution could appear small with respect to the overall objective; however, it is clear that a manifold of technologies will contribute to the transition phase and do its part. Moreover, the implementation of the TCR-PSA-HDO combined system is here evaluated only with respect to the availability of sewage sludge, but other residues or biomass waste can be involved and evaluated as well.

## 6.2 Considerations for the modelling framework

### 6.2.1 Strengths and limitations

The modelling framework was developed in the attempt to relax certain fixed assumptions of the conventional LCA, which would not be realistic for measuring the environmental consequences of an action which unfolds over a large time frame. Through the case study it was showed that within this framework the following features have the potential to be modelled:

- Structural changes in the economy (coefficients in matrix  $A$ ), such as the gradual change over time of the electricity mix due to the transition to renewable energy.
- The implementation of a novel technology, considering its gradual market penetration and the corresponding actual scale.
- Changes in the marginal technologies (both for substituted functions and intermediate products) at the foreground system level, for instance the technology affected by the TSF Phosphorus

production is initially the P-fertilisers sector in EU-28, and subsequently a mix of P-fertilisers sector in EU-28 and the corresponding sector in RoW.

Other possible features were not taken into consideration for this case study, but have the potential to be included as well, which include:

- Changes over time in the environmental stressors associated to each sector (coefficients in matrix **B**), for example due to improved efficiency of industrial processes.
- Changes over time in background environmental systems affecting the characterisation factors (matrix **C**), for example due to different background concentrations in environmental compartments.
- Unperfect substitution between new products and alternatives, for example an increase of final demand for fuels due to the additional supply of biofuels.
- Economies of scale and learning curves applied for modelling system-specific changes in the foreground parameters.
- Feedback effects between the economic and the environmental system; indeed, the system dynamics modelling environment allows to model interdependencies between the two systems which are not interconnected in a conventional LCA modelling structure.

Moreover, the system dynamics environment allows for the coupling with causal dynamic models that can generate the array coefficients instead of considering pre-established scenarios, such as the ones by the IEA used for this case study.

At the basis of this framework there is the consequential thinking according to which the decision context is tested against a counterfactual, i.e. the outcomes that would have occurred in the absence of the decision (further discussed in section 6.2.3). The explicit modelling of a counterfactual scenario is rarely considered in the consequential framework, since usually only a change in demand is modelled (and consequently its effects), without the need to explicitly model two situations to be compared, i.e. with and without the decision. The most similar work which follows this approach, as the proposed framework, is the study by Menten et al. (2015) [102], which analyses the consequences of the future production in France of a second-generation biofuel. Differently from the presented case study, it considers limited system boundaries, since it aims at the identification of affected technologies only in the French energy and transportation sectors, thus excluding consequences on international markets and domestic non-energy markets. However, in a similar way, it models both the scenario with the novel technology implementation and the “no decision” scenario, where their impact difference represents the “environmental consequences”; moreover, it considers two possible

policy options, one including environmental targets and one other without political constraints. Their results confirm even more that the policy context is particularly relevant for the environmental consequences of the implemented technology, since the technologies impacted by the decision are not the same under the two policies; finally, it also confirms that the environmental benefits of a “green” technology are generally lower in a more ambitious policy context.

However, not considering international trade and effects on non-energy related sectors can be regarded as a clear limitation: the authors of the above-mentioned work recognise that potentially important system effects are neglected, due to the limited geographical and sectoral coverage of their model [102].

To overcome the problem of limited system boundaries, the present framework proposes the combination of process LCA for the foreground system and IO analysis for the background system. On the other hand, the rough aggregation into two regions and a limited number of economic sectors can determine the loss of technological details which can have a certain relevance on the environmental outcomes. For example, while the role of chemicals in the present study appeared to give an important contribution to the impacts, it was not possible to distinguish between different types of chemical products which would presumably be produced with very different impacts. Nonetheless, this limitation can be overcome extending the detailed process-based data to a second tier beyond the first tier of the foreground system.

Furthermore, IO models share with LCA models other shortcomings, concerning the linear structure and the assumption of unlimited supply of inputs. However, in this regard it can be said that the dynamic modelling of the IO structure represents a step forward with respect to the fixed input/output relationships, allowing to introduce exogenously substitution of inputs and shifts in the use of energy resources [103]. Similar approaches for the dynamical modelling through the modification of technical coefficients in the IO matrices can be found in recent studies, such as Hertwich et al. (2015) [104]. Nevertheless, these techniques are normally used to assess the global impacts of a structural change, such as the shift to renewable energy, i.e. they assess how different policy and energy scenarios perform differently by itself, rather than assessing a specific technology or decision in the context of the prospected scenarios.

Another limit of the present framework, connected to the absence of supply constraints, is the inability to model land use change effects, which is often a relevant aspect to consider in the analysis of bioenergy technologies [105]. However, land use change in the present study was not considered a key topic, since the feedstock of the novel technology is waste biomass, which should not increase the need for land. Another possible effect not captured by the IO model, is the one concerning the

change in soil properties due to the avoided land spreading of sewage sludge. In this regard, it should be noticed that land spreading of sewage sludge, due to the presence of pollutants, is a practice currently not allowed in some states and it is expected to be banned elsewhere in the coming years. In a certain sense, it is not an environmental consequence to be ascribed to the TSF technology; if anything, it would require a revision of the counterfactual scenario, to account for a growth in the incineration (or landfilling) sector and a degrowth in the land application sector.

## 6.2.2 Relevance of the context

Most of the environmental quantitative assessments consider the environmental performance of a product as an intrinsic property of it. For instance, from the RED regulation [106] it could be deduced that GWP is a property of a fuel. Although this assumption may be acceptable in some cases, in the attempt to simplify a reality otherwise too complex to be analysed in a structured analysis, in other situations it can lead to misleading results. The proposed framework starts from the consideration that the environmental consequences of choosing to rely on a specific technology, for example in the field of bioenergy, depend on factors that cannot be left out of the analysis. These are represented by the scale of technology implementation and the technological, economic and policy context. This especially concerns situations where a long-term perspective is considered and, consequently, the variability of the context can play a key role. It should be clear that, for example, a choice on which type of energy supply to rely on in the coming decades cannot be treated in the same way as a small consumer choice in the very short term.

There is a need to develop prospective assessment models, in which possible future contexts are outlined on the basis of scenarios constructed by economists and other experts from different disciplines. In particular, energy scenarios can have an important role in the environmental profile of many products [107]. For this reason, this study was focused on the use of possible electricity scenarios, as outlined by a globally recognised source such as the IEA, whereas for all other sectors, in practice, current situation was used as a proxy for future situations. However, the same approach could be applied to any sector likely to face important changes in the future. The proposed framework is conceived for the integration in a hybrid LCA of external prospective models that make projections about future technological and environmental changes. In the presented case study, data series generated outside the model were used, but the system dynamics environment potentially allows for hardlinking with prospective models that can directly modify the LCA matrix coefficients.

At the same time, it is clear that predicting the future with perfect accuracy is impossible and all prospective models have limitations. Nevertheless, these tools should become common practice in the attempt to provide a context to support strategic decisions and underline the relative nature of quantitative assessment, that any policy-maker should always keep in mind.

### 6.2.3 The reference system or the counterfactual

The concept of reference situation is often disregarded in LCA, although it is a key issue in comparative analyses. Baseline scenario, reference scenario, reference system, business-as-usual and counterfactual are used often as synonyms, other times with different meanings. In particular, two concepts are used ambiguously and frequently associated: “reference system” and “counterfactual”. The reference system is usually considered in ALCA studies to compare the results of the studied system with other systems, while the counterfactual is the zero-option or business-as-usual against which to measure the consequences of a decision in a CLCA. However, also in CLCA a proper counterfactual is rarely explicitly modelled, in practice assuming that the system under study, in the absence of the decision, would remain unchanged or static [39].

The reference system for ALCA represents an implicit counterfactual for final products [42]. Cherubini & Strømman (2011) [72] observe that most studies of biomass-to-energy systems have a fossil system as reference, some others have alternative biomass systems (e.g. old stoves using wood vs. new stoves using wood, or 1<sup>st</sup> generation bioethanol vs. 2<sup>nd</sup> generation bioethanol) and a few ones have none. It seems that the intended purpose behind the choice of the reference system is not the same among practitioners. The research question could be: “which is the system that would be replaced by the new one?” Or could be also: “which is the system that could be used as baseline for evaluating the new system?” It is not clear which is the research question in the case studies analysed and which meaning is given to the reference system. The first question follows more a consequential logic, while the second question seems appropriate for an attributional approach. However, a consequential logic should also consider other consequences than the simple replacement of a “new” system with an “old” one. For this reason, it should be more appropriate in a consequential approach to assess a decision (which would imply, among other things, the substitution of a somehow “old” product supply-chain with the “new” product supply-chain) against a counterfactual, intending not a reference (or “alternative”) system, but more generally a situation in which the decision does not take place. The narrow question “Which is the system that would be replaced by the new one?” in this case would be changed in the more comprehensive question “How the world (without the decision),

that would be replaced by the “new” one (with the decision), would look like?”. The latter question includes the first question, to some extent, since a decision usually involves a new system which could replace an older or alternative system. But the latter question is more open and call for a modelling effort much bigger, more focused on the dynamics of wide systems than strictly on the products life cycles. In a certain sense, this type of analysis can become something considerably more extended (and different) than what was originally intended with life cycle assessment.

The proposed framework, grasping this need, includes the explicit modelling of the counterfactual “no decision” scenario. The final products supplied by the biorefinery, in this way, do not need to be individually compared with reference products produced in other (reference) systems: the substitution of certain other products (modelled through “substitution factors”) is considered as a consequence of their production by the biorefinery, of equal importance with respect to other dynamics that can be modeled starting from the decision.

#### 6.2.4 Functional unit definition when assessing decisions

When modelling the consequences of large-scale decisions, it is recommended to choose a functional unit of the same size as the decision to be supported by the study [108]. However, it can be argued that, in this way, the original purpose of the functional unit would be lost, since the possibilities to compare the studied system with other options would be very limited.

The importance of the choice of the functional unit in the LCA framework is connected to the need of comparability. A product system is assumed “interchangeable” with another one if they fulfil the same function. The functional unit defines the quantification of the identified functions (performance characteristics), which is necessary to ensure the comparability of results among studies. In this way, it is possible to describe two (or more) systems which are equivalent, fulfilling the same function to the same extent. When two alternative systems are assessed, their impacts are ultimately compared to understand which is the best way, from an environmental point of view, to provide a certain function. However, if the object of the assessment is not a product but a decision, it is difficult to define a function, and probably it is not necessary, since the outcomes of the assessment of a decision should have a value by itself. The decision could be referred as “substituting refineries with biorefineries”, or “installing X plants which will produce Y tons of transport fuels from biomass feedstock”. For instance, the analysis of this case study considered the latter type of decision, and it showed that environmental advantages can be obtained if the biorefinery system is implemented. Instead, the outcomes of the assessment of a product would consist in declaring the environmental

impacts associated to that product (e.g. a biofuel), and only subsequently comparing its environmental performance to that of another product used as a reference (e.g. a conventional fuel). In product LCA, different ways to fulfil defined functions are ultimately assessed. The function can be “driving” or “fuel production”. However, assessing a decision can be a very different exercise. Another example could be the policy decision to introduce a carbon tax. What is the function of this decision? It is clear that changes in consumer behaviour would take place, therefore no functional equivalence would stand between the decision scenario and the zero option. Indeed, traditional LCA does not consider the zero option, since it would imply a change in function.

The shift from a close focus on single product systems to the more generally wider systems for large decisions, also questions the use of the functional unit. In the consequential approach, two systems (or situations) are compared, which are not necessarily functionally equivalent. The system boundaries are expanded so as to include any activity which is expected to change as a consequence of the decision at hand. In doing so, as noticed by *Zamagni et al. (2012)* [38], “the resulting functional unit of the whole system would consist of multiple functions, including the main system and those added by the processes included in the boundaries”. *Zamagni et al. (2012)* also notice: “When a comparative analysis has to be conducted, it might be difficult to guarantee the functional equivalency between the systems compared, since the processes included in the two situations might serve different functions”. Indeed, if the goal is to capture the broader environmental consequences of the decision at hand, these could include, for example, price effects determining the decrease in price for transport fuels, thus people might decide to drive more. Or, further on, the increased use in biomass could determine land use changes which will in turn determine an increase in the price of food, in such a manner that consumption choices of world population might be forced to change. In this case, the comparison is not simply between a world in which a certain amount of “driving” is derived from biomass technologies and a world in which the same amount is derived from fossil fuel technologies (while everything else stands equal). The comparison would be between two situations with possible differences in total consumption patterns, both for products directly related to the decision (transport fuels), and for products indirectly affected (e.g. food). Such analyses do not require a functional unit, since no functional equivalence would stand between the two situations. It should be also pondered if it is appropriate to model such indirect effects in the context of life cycle analysis, or it would be better to limit LCA to its close focus on single product systems and delegate the analysis of possible rebound effects (on other product system, or economies and society) to other types of sustainability tools.



*Weidema (2003)* [40] has also affirmed that: “As attributional LCA does not apply to comparison of alternative product systems, the functional unit does not play any important role for the assessment, and may therefore be chosen at will”. While this statement is not exactly true (an attributional LCA does not apply comparison, but it involves comparisons when different studies are compared on the basis of their functional unit), it contains an important but disregarded consideration: the functional unit is useful just for comparative purposes, therefore if there are no comparisons involved, the functional unit is not necessary anymore. Hence, at the opposite it could be concluded that the functional unit does not play any important role for a consequential assessment which incorporates the comparison of two alternatives, namely the “decision” scenario and the “no decision” scenario, and its results are not necessarily meant for further comparisons, just showing the environmental consequences of a certain decision. The decision could involve new products, as in the case of the studied biorefinery system, which would come on stage substituting other functions already fulfilled by pre-existing products. Each of these products can be substituted with the new ones on the basis of the principle of functional equivalence, e.g. a new biofuel should provide the same amount of function (“driving”) of the fuels substituted. The same applies for co-product which could come on stage along the supply-chain and the system investigated in general. Indeed, by doing so, the functional equivalence would still represent a fundamental principle for building the studied system.

In conclusion, improving the applications of CLCA should start from clearly stating the decision (equally important of clearly stating the functional unit for a ALCA). The function (and the functional unit) should be indicated if reasonable options to the decision exists. For this reason, the present case study was analysed without declaring a functional unit. If for large decisions a functional unit is requested of the same size as the decision, its definition should be straightforward once the decision is clearly stated. Nevertheless, it was still useful to refer to a production unit (in terms of revenues) to compare the performance of the technology over the time frame of the analysis, since the production volume was not constant over time. This unit was used for internal comparison of the same biorefinery system operating in different years or contexts, and it should not be confused with the functional unit.

# 7 Conclusions

This thesis work started from the need to evaluate the environmental sustainability of an emerging technology in the field of bioenergy, and its potential for contributing to the transition phase from fossil fuels towards renewable sources, through its implementation at large scale in European Union. Indeed, EU has currently the ambitious target to reach climate neutrality by 2050. Life cycle assessment is the standard tool used for the environmental assessment of product-related systems, and thus appears as the most appropriate reference tool to use in such a situation. At the same time, LCA methodology is acknowledged having some important limitations, and is still going through a phase of research and development in the scientific community. Indeed, it is characterised by assumptions and simplifications that, while being certainly useful in reducing the complexity of the analysis and easing its applicability, are often considered too limiting, in particular when it is used for evaluating technologies which are intended for development on a large scale and promise to have high impacts on the economy and society.

The analysed emerging technology, represented by the TCR-PSA-HDO combined process, has all the characteristics to be ascribed in the category of biorefinery systems: it is an integrated process for refining biomass into many products in a novel and efficient way, and it is likely to be environmentally advantageous. Indeed, its products are expected to displace especially fossil fuels and avoid their related harm on the environment. However, from an LCA viewpoint this type of system poses a relevant challenge, since it represents the typical multifunctional situation which requires consistent criteria to ascribe process requirements to each function provided by the coproduction process. Moreover, the use of waste biomass (sewage sludge) as feedstock implies that the studied multi-functional process has both functional outflows and inflows: in addition to the product-related functions, it also provides a waste management function; this aspect adds up to the complexity for handling multifunctionality.

The project To-Syn-Fuel, aiming at the demonstration of the TCR-PSA-HDO combined system with an advancement from TRL-5 to TRL-7, includes the evaluation of the environmental sustainability, which is performed through a conventional LCA in compliance with ISO standards. Furthermore, the

RED regulation imposes for biofuels and bioenergy products, obtained through the technology, the achievement of specific targets of “GHG savings” compared with fossil equivalents: these requirements oblige the analysis to assume a product-oriented approach and evaluate the system from the perspective of fuel production. Conversely, the present thesis work points to the overarching challenge of capturing the environmental consequences of the decision to implement the technology according to the plans for its future market deployment prospected in the To-Syn-Fuel project. The review on the advancements on the LCA research suggested that the conventional framework is suboptimal for this type of research questions. Specifically, the analysis should be change-oriented, able to capture the broader environmental consequences of the decision, and include a long-term perspective, considering for example changes in boundary conditions or in technological and regulatory contexts that are expected to take place in the future. For this reason, the present study proposes a different framework for an LCA-based analysis, which can provide a flexible structure where all these aspects can be considered; in particular, it can allow to relax certain fixed assumptions of the static LCA, which would be not realistic for measuring the environmental consequences of a decision which unfolds over a large time frame. Furthermore, within this framework it is not necessary to focus on a specific function: the technology is analysed comprehensively, considering the whole set of functions provided and the consequences of each of them in terms of substitution of alternative products in the economic system. This is possible since results are not meant to be used in comparative analysis with other systems on the basis of a functional equivalence (e.g. as requested by the RED regulation). On the other hand, a comparison is rarely feasible when modelling the consequences of large-scale decisions, for which is generally recommended to choose a functional unit of the same size of the decision supported by the study. On the contrary, the results of the present study are meant to provide a best estimate of impact savings associated with the decision. In order to do this, the proposed framework included the explicit modelling of two situations, one simulating a system with the decision taking place and one other simulating the same system without the decision. Indeed, the results were presented in terms of change in impacts between the two situations, and they do not require further comparisons. For this type of evaluation, terms such as "GHG savings" would be used more appropriately, since the framework acknowledges that the savings are not necessarily the simple difference between the respective impacts associated to two (or more) alternative products, but they are the result of systemic changes which also includes substitution between alternative products.

The proposed framework also acknowledges the relevance of the context on the results of an environmental assessment. Indeed, the same technology, set in different contexts, may lead to

different environmental consequences. With the purpose of taking the specific context into due account, wide boundaries are considered, and a prospective assessment is adopted. From a practical viewpoint, a dynamic hybrid input-output table was built, reflecting the gradual implementation of the technology over time and the evolution of future energy scenarios. The results showed how the variability of the context can lead to affect differently other sectors in the economy, even the ones which are not directly interconnected to the new technology; this was the case, for example, of the coal electricity sector, which had a relevant influence on final environmental outcomes. The variability of the context was considered both in terms of change over time and different possible scenarios.

Finally, the assessment proved to be able in providing a clear and not ambiguous way for measuring the contribution of a specific decision to more general environmental targets fixed by policy makers. The conventional LCA framework is still valid and useful for decision-making support, providing a first evaluation of a novel technology based on product comparison. However, before its deployment at commercial scale, the full effects of the supported decision should be evaluated. In the hope for the development of new standardised modelling frameworks, including commonly-shared scenarios and criteria for key methodological choices, the present framework was proposed as an attempt to show a possible direction.

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# 8 Supplementary material

## 8.1 EXIOBASE aggregation tables

Number	Name	Aggregation
1	Paddy rice	Agriculture,Forestry,Fishing
2	Wheat	Agriculture,Forestry,Fishing
3	Cereal grains nec	Agriculture,Forestry,Fishing
4	Vegetables, fruit, nuts	Agriculture,Forestry,Fishing
5	Oil seeds	Agriculture,Forestry,Fishing
6	Sugar cane, sugar beet	Agriculture,Forestry,Fishing
7	Plant-based fibers	Agriculture,Forestry,Fishing
8	Crops nec	Agriculture,Forestry,Fishing
9	Cattle	Agriculture,Forestry,Fishing
10	Pigs	Agriculture,Forestry,Fishing
11	Poultry	Agriculture,Forestry,Fishing
12	Meat animals nec	Agriculture,Forestry,Fishing
13	Animal products nec	Agriculture,Forestry,Fishing
14	Raw milk	Agriculture,Forestry,Fishing
15	Wool, silk-worm cocoons	Agriculture,Forestry,Fishing
16	Manure (conventional treatment)	Agriculture,Forestry,Fishing
17	Manure (biogas treatment)	Agriculture,Forestry,Fishing
18	Products of forestry, logging and related services (02)	Agriculture,Forestry,Fishing
19	Fish and other fishing products; services incidental of fishing (05)	Agriculture,Forestry,Fishing
20	Anthracite	Energy
21	Coking Coal	Energy
22	Other Bituminous Coal	Energy
23	Sub-Bituminous Coal	Energy
24	Patent Fuel	Energy
25	Lignite/Brown Coal	Energy
26	BKB/Peat Briquettes	Energy
27	Peat	Energy
28	Crude petroleum and services related to crude oil extraction, excluding surveying	Energy
29	Natural gas and services related to natural gas extraction, excluding surveying	Natural gas
30	Natural Gas Liquids	Energy
31	Other Hydrocarbons	Energy
32	Uranium and thorium ores (12)	Energy
33	Iron ores	Industry
34	Copper ores and concentrates	Industry
35	Nickel ores and concentrates	Industry
36	Aluminium ores and concentrates	Industry
37	Precious metal ores and concentrates	Industry
38	Lead, zinc and tin ores and concentrates	Industry
39	Other non-ferrous metal ores and concentrates	Industry
40	Stone	Industry
41	Sand and clay	Industry
42	Chemical and fertilizer minerals, salt and other mining and quarrying products n.e.c.	Industry
43	Products of meat cattle	Agriculture,Forestry,Fishing
44	Products of meat pigs	Agriculture,Forestry,Fishing
45	Products of meat poultry	Agriculture,Forestry,Fishing



46	Meat products nec	Agriculture,Forestry,Fishing
47	products of Vegetable oils and fats	Agriculture,Forestry,Fishing
48	Dairy products	Agriculture,Forestry,Fishing
49	Processed rice	Agriculture,Forestry,Fishing
50	Sugar	Agriculture,Forestry,Fishing
51	Food products nec	Agriculture,Forestry,Fishing
52	Beverages	Agriculture,Forestry,Fishing
53	Fish products	Agriculture,Forestry,Fishing
54	Tobacco products (16)	Industry
55	Textiles (17)	Industry
56	Wearing apparel; furs (18)	Industry
57	Leather and leather products (19)	Industry
58	Wood and products of wood and cork (except furniture); articles of straw and plaiting materials (20)	Industry
59	Wood material for treatment, Re-processing of secondary wood material into new wood material	Industry
60	Pulp	Industry
61	Secondary paper for treatment, Re-processing of secondary paper into new pulp	Industry
62	Paper and paper products	Industry
63	Printed matter and recorded media (22)	Industry
64	Coke Oven Coke	Energy
65	Gas Coke	Energy
66	Coal Tar	Energy
67	Motor Gasoline	Motor Gasoline
68	Aviation Gasoline	Energy
69	Gasoline Type Jet Fuel	Energy
70	Kerosene Type Jet Fuel	Energy
71	Kerosene	Energy
72	Gas/Diesel Oil	Diesel Oil
73	Heavy Fuel Oil	Energy
74	Refinery Gas	Energy
75	Liquefied Petroleum Gases (LPG)	Energy
76	Refinery Feedstocks	Refinery Feedstocks
77	Ethane	Energy
78	Naphtha	Energy
79	White Spirit & SBP	Energy
80	Lubricants	Lubricants
81	Bitumen	Energy
82	Paraffin Waxes	Energy
83	Petroleum Coke	Energy
84	Non-specified Petroleum Products	Energy
85	Nuclear fuel	Energy
86	Plastics, basic	Industry
87	Secondary plastic for treatment, Re-processing of secondary plastic into new plastic	Industry
88	N-fertiliser	Industry
89	P- and other fertiliser	P fertilisers
90	Chemicals nec	Chemicals
91	Charcoal	Energy
92	Additives/Blending Components	Energy
93	Biogasoline	Biogasoline
94	Biodiesels	Biodiesels
95	Other Liquid Biofuels	Energy
96	Rubber and plastic products (25)	Industry
97	Glass and glass products	Industry
98	Secondary glass for treatment, Re-processing of secondary glass into new glass	Industry
99	Ceramic goods	Industry
100	Bricks, tiles and construction products, in baked clay	Industry
101	Cement, lime and plaster	Cement,Lime and Plaster
102	Ash for treatment, Re-processing of ash into clinker	Industry
103	Other non-metallic mineral products	Industry
104	Basic iron and steel and of ferro-alloys and first products thereof	Iron and Steel
105	Secondary steel for treatment, Re-processing of secondary steel into new steel	Industry

<b>106</b>	Precious metals	Industry
<b>107</b>	Secondary precious metals for treatment, Re-processing of secondary precious metals into new precious metals	Industry
<b>108</b>	Aluminium and aluminium products	Aluminium
<b>109</b>	Secondary aluminium for treatment, Re-processing of secondary aluminium into new aluminium	Industry
<b>110</b>	Lead, zinc and tin and products thereof	Industry
<b>111</b>	Secondary lead for treatment, Re-processing of secondary lead into new lead	Industry
<b>112</b>	Copper products	Copper
<b>113</b>	Secondary copper for treatment, Re-processing of secondary copper into new copper	Industry
<b>114</b>	Other non-ferrous metal products	Industry
<b>115</b>	Secondary other non-ferrous metals for treatment, Re-processing of secondary other non-ferrous metals into new other non-ferrous metals	Industry
<b>116</b>	Foundry work services	Industry
<b>117</b>	Fabricated metal products, except machinery and equipment (28)	Industry
<b>118</b>	Machinery and equipment n.e.c. (29)	Industry
<b>119</b>	Office machinery and computers (30)	Industry
<b>120</b>	Electrical machinery and apparatus n.e.c. (31)	Industry
<b>121</b>	Radio, television and communication equipment and apparatus (32)	Industry
<b>122</b>	Medical, precision and optical instruments, watches and clocks (33)	Industry
<b>123</b>	Motor vehicles, trailers and semi-trailers (34)	Industry
<b>124</b>	Other transport equipment (35)	Industry
<b>125</b>	Furniture; other manufactured goods n.e.c. (36)	Industry
<b>126</b>	Secondary raw materials	Industry
<b>127</b>	Bottles for treatment, Recycling of bottles by direct reuse	Industry
<b>128</b>	Electricity by coal	Electricity(Coal)
<b>129</b>	Electricity by gas	Electricity(Gas)
<b>130</b>	Electricity by nuclear	Electricity(Nuclear)
<b>131</b>	Electricity by hydro	Electricity(Hydro)
<b>132</b>	Electricity by wind	Electricity(Wind)
<b>133</b>	Electricity by petroleum and other oil derivatives	Electricity(Petroleum)
<b>134</b>	Electricity by biomass and waste	Electricity(Biomass and Waste)
<b>135</b>	Electricity by solar photovoltaic	Electricity(Solar PV)
<b>136</b>	Electricity by solar thermal	Electricity(Solar Thermal)
<b>137</b>	Electricity by tide, wave, ocean	Electricity(Tide,Wave,Ocean)
<b>138</b>	Electricity by Geothermal	Electricity(Geothermal)
<b>139</b>	Electricity nec	Electricity(other)
<b>140</b>	Transmission services of electricity	Energy
<b>141</b>	Distribution and trade services of electricity	Energy
<b>142</b>	Coke oven gas	Energy
<b>143</b>	Blast Furnace Gas	Energy
<b>144</b>	Oxygen Steel Furnace Gas	Energy
<b>145</b>	Gas Works Gas	Energy
<b>146</b>	Biogas	Energy
<b>147</b>	Distribution services of gaseous fuels through mains	Energy
<b>148</b>	Steam and hot water supply services	Steam and Hot Water
<b>149</b>	Collected and purified water, distribution services of water (41)	Collected and Purified Water
<b>150</b>	Construction work (45)	Industry
<b>151</b>	Secondary construction material for treatment, Re-processing of secondary construction material into aggregates	Industry
<b>152</b>	Sale, maintenance, repair of motor vehicles, motor vehicles parts, motorcycles, motor cycles parts and accessories	Services
<b>153</b>	Retail trade services of motor fuel	Services
<b>154</b>	Wholesale trade and commission trade services, except of motor vehicles and motorcycles (51)	Services
<b>155</b>	Retail trade services, except of motor vehicles and motorcycles; repair services of personal and household goods (52)	Services
<b>156</b>	Hotel and restaurant services (55)	Services
<b>157</b>	Railway transportation services	Railway Transportation
<b>158</b>	Other land transportation services	Other Land Transportation
<b>159</b>	Transportation services via pipelines	Services

<b>160</b>	Sea and coastal water transportation services	Services
<b>161</b>	Inland water transportation services	Services
<b>162</b>	Air transport services (62)	Services
<b>163</b>	Supporting and auxiliary transport services; travel agency services (63)	Services
<b>164</b>	Post and telecommunication services (64)	Services
<b>165</b>	Financial intermediation services, except insurance and pension funding services (65)	Services
<b>166</b>	Insurance and pension funding services, except compulsory social security services (66)	Services
<b>167</b>	Services auxiliary to financial intermediation (67)	Services
<b>168</b>	Real estate services (70)	Services
<b>169</b>	Renting services of machinery and equipment without operator and of personal and household goods (71)	Services
<b>170</b>	Computer and related services (72)	Services
<b>171</b>	Research and development services (73)	Services
<b>172</b>	Other business services (74)	Services
<b>173</b>	Public administration and defence services; compulsory social security services (75)	Services
<b>174</b>	Education services (80)	Services
<b>175</b>	Health and social work services (85)	Services
<b>176</b>	Food waste for treatment: incineration	Waste Management
<b>177</b>	Paper waste for treatment: incineration	Waste Management
<b>178</b>	Plastic waste for treatment: incineration	Waste Management
<b>179</b>	Inert/metal waste for treatment: incineration	Inert Waste Incineration
<b>180</b>	Textiles waste for treatment: incineration	Waste Management
<b>181</b>	Wood waste for treatment: incineration	Waste Management
<b>182</b>	Oil/hazardous waste for treatment: incineration	Waste Management
<b>183</b>	Food waste for treatment: biogasification and land application	Waste Management
<b>184</b>	Paper waste for treatment: biogasification and land application	Waste Management
<b>185</b>	Sewage sludge for treatment: biogasification and land application	Sewage Sludge Land Application
<b>186</b>	Food waste for treatment: composting and land application	Waste Management
<b>187</b>	Paper and wood waste for treatment: composting and land application	Waste Management
<b>188</b>	Food waste for treatment: waste water treatment	Waste Management
<b>189</b>	Other waste for treatment: waste water treatment	Waste Water Treatment
<b>190</b>	Food waste for treatment: landfill	Waste Management
<b>191</b>	Paper for treatment: landfill	Waste Management
<b>192</b>	Plastic waste for treatment: landfill	Waste Management
<b>193</b>	Inert/metal/hazardous waste for treatment: landfill	Inert Waste Landfill
<b>194</b>	Textiles waste for treatment: landfill	Waste Management
<b>195</b>	Wood waste for treatment: landfill	Waste Management
<b>196</b>	Membership organisation services n.e.c. (91)	Services
<b>197</b>	Recreational, cultural and sporting services (92)	Services
<b>198</b>	Other services (93)	Services
<b>199</b>	Private households with employed persons (95)	Services
<b>200</b>	Extra-territorial organizations and bodies	Services

## 8.2 Code repository

```
import pymrio as mr
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.lines as mlines
import matplotlib.transforms as mtransforms
import os
import pandas as pd
os.chdir("/Desktop/IOT")
folder = 'IOT_2011_pxp'
pxp = mr.load_all(path = folder)
pxp.meta
pxp.calc_all()
reg_agg_vec = ['EU28' if i<28 else 'RoW' for i,r in
enumerate(pxp.get_regions())]
products = pd.read_csv(os.path.join(folder,'products.txt'),
sep='\t',index_col=0)
products['2-digit code'] = products.CodeNr.str[1:3]
sec_agg = pd.read_excel('aggregation-by product.xlsx').iloc[:,1:]
sec_agg_vec = sec_agg['Aggregation'].values
pxp_agg =
pxp.aggregate(sector_agg=sec_agg_vec,region_agg=reg_agg_vec,inplace=False)
pxp_agg.calc_all()
pxp_agg.x.sum(), pxp.x.sum()
pxp.x
pxp_agg.save_all('pxp_EU_RoW2011')
```

## 8.3 Characterisation factors

		GWP (100years)	POCP	AP	EP	HTP
		kg CO2 eq	kg C2H4 eq	kg SO2 eq	kg PO4--- eq	kg 1,4-DB eq
CO2 - combustion	kg	1	0	0	0	0
CH4 - combustion	kg	25	0.006	0	0	0
N2O - combustion	kg	298	0	0	0.27	0
SOx - combustion	kg	0	0.048	1.2	0	0.096
NOx - combustion	kg	0	0	0.5	0.13	1.2
NH3 - combustion	kg	0	0	1.6	0.35	0.1
CO - combustion	kg	0	0.027	0	0	0
PCDD_F - combustion	kg I-TEQ	0	0	0	0	1933982792
HCB - combustion	kg	0	0	0	0	3157103.03
NMVOC - combustion	kg	0	0	0	0	11.40074339
PM10 - combustion	kg	0	0	0	0	0.82
As - combustion	kg	0	0	0	0	347699.6973
Cd - combustion	kg	0	0	0	0	145040.5399
Cr - combustion	kg	0	0	0	0	646.8397982
Cu - combustion	kg	0	0	0	0	4295.027793
Hg - combustion	kg	0	0	0	0	6008.157802
Ni - combustion	kg	0	0	0	0	35032.83874
Pb - combustion	kg	0	0	0	0	466.517307
Se - combustion	kg	0	0	0	0	47687.15468
Zn - combustion	kg	0	0	0	0	104.4419271
CO2 - non combustion	kg	1	0	0	0	0
CH4 - non combustion	kg	25	0.006	0	0	0
N2O - non combustion	kg	298	0	0	0.27	0
SOx - non combustion	kg	0	0.048	1.2	0	0.096
NOx - non combustion	kg	0	0	0.5	0.13	1.2
NH3 - non combustion	kg	0	0	1.6	0.35	0.1
CO - non combustion	kg	0	0.027	0	0	0
PAH - non combustion	kg	0	0	0	0	199567.4997
PCDD_F - non combustion	kg I-TEQ	0	0	0	0	1933982792
HCB - non combustion	kg	0	0	0	0	3157103.03
NMVOC - non combustion	kg	0	0	0	0	11.40074339
PM10 - non combustion	kg	0	0	0	0	0.82
As - non combustion	kg	0	0	0	0	347699.6973
Cd - non combustion	kg	0	0	0	0	145040.5399

Cr - non combustion	kg	0	0	0	0	646.8397982
Cu - non combustion	kg	0	0	0	0	4295.027793
Hg - non combustion	kg	0	0	0	0	6008.157802
Ni - non combustion	kg	0	0	0	0	35032.83874
Pb - non combustion	kg	0	0	0	0	466.517307
Se - non combustion	kg	0	0	0	0	47687.15468
Zn - non combustion	kg	0	0	0	0	104.4419271
SF6	kg	22800	0	0	0	0