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Integration of sustainability paradigms in the evaluation of energy scenarios

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Abstract

The awareness matured in recent years towards the necessity of climate change mitigation is leading to a change in priorities across all the sectors of the economy, especially in industrial production and power generation. The current paradigm in place for the solution of the problem is mostly focused towards the abatement of greenhouse gases emissions. Nonetheless, from a social and economic perspective, a sharp transition could bring non-negligible issues in terms of energy reliability and affordability. In this context, the relevance of computer-aided techniques, such as energy system models, plays a crucial role. The goal behind large part of the energy system models is to provide a set of least-cost solutions for the development of the technology mix to achieve prescribed environmental targets, such as CO₂ emission reduction. Several aspects, like environmental footprint, energy security and human health risks, are completely unaccounted for in the currently existing modelling frameworks. Each of those aspects requires the accounting of several dimensions that can fall inside the wide definition of sustainability. The aim of this thesis is dual. First of all, a metric for the evaluation of the overall sustainability level of an energy scenario is proposed. Given the trend towards an ever-higher electrification of energy end-uses, the work has been concentrated on the power sector. All the modelled technologies were characterized by a set of parameters regarding life cycle impacts and other energy issues-related indicators. Those parameters and their ability to represent the system sustainability are validated with several simulations coming from the TIMES bottom-up energy model generator, achieving higher scores for low carbon scenarios. The second goal of this work is to improve the traditional energy system modeling paradigm based on emission-constrained economic, shifting it from a mainly economic-oriented algorithm to a combined sustainability-economic optimization. The same sustainability metrics applied ex-post in the previous phase has been endogenously integrated, accounting for that either as a model constraint or as a component of the final objective function. In this multi-objective optimization context, the user has the possibility to decide the level of priority of the two components, thanks to a weighted sum approach. Results show how it is possible to prioritize the sustainability evaluation of the scenarios limiting the economic expenditure, thanks to an optimized configuration of the energy mix. Moreover, it is possible to highlight the role of the different energy technologies in modifying the sustainability of an energy scenario. Further steps may be the application of the modified version of the model to more complex models and the integration of this innovative approach in all the other modelled sectors.

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List of acronyms

AF	Availability Factor
CF	Capacity Factor
CPLEX	IBM ILOG CPLEX Optimization Studio
ETM	EUROfusion TIMES Model
EU	European Union
GAMS	General Algebraic Modeling System
GDP	Gross domestic product
GHG	Greenhouse gases
GLPK	GNU Linear Programming Kit
IAEA	International Atomic Energy Agency
IEA	International Energy Agency
LCA	Life cycle assessment
LCIA	Life cycle impact assessment
MCDA	Multi Criteria Decision Analysis
MOO	Multi objective optimization
NEOS	Network-Enabled Optimization System
O&M	Operation and maintenance
RES	Reference energy system
TEMOA	Tools for Energy Modeling Optimization and Analysis
TIMES	The Integrated MARKAL-EFOM System
TRL	Technology readiness level
UK	United Kingdom
VARO&M	Variable operation and maintenance
VEDA	Versatile Data Analyst

Chapter 1: Introduction

Interest in combining technological development and economic growth in such a way that is compatible with the ecosystem in which human beings are inserted is not a recent topic. Indeed, already in 1972, with the famous report “The limits to growth” published by The Club of Rome [1], the constraint of the anthropic pressure imposed by the finite resource environment in which we are inserted have been discussed. In particular, the authors analyzed different global scenarios, each of them characterized by several economic and population growth assumptions. The analysis was focused on four factors that determine and ultimately limit economic growth on the planet: population increase, agricultural production, non-renewable resource depletion, industrial output, and pollution generation. In this framework the focus was on achieving a state of global equilibrium with population and production in carefully selected balance.

It is possible to define in a very general way the concept of sustainability that will drive this analysis. In its wider formulation, the sustainability of a certain system can be intended as the configuration that guarantee both a short and a long-term equilibrium between the system and its surrounding environment [1]. The main issue when talking about sustainability rely on its definition, which is very case specific. This also justify the high number of scientific works related to this topic published in the last years, as shown in Figure 1.

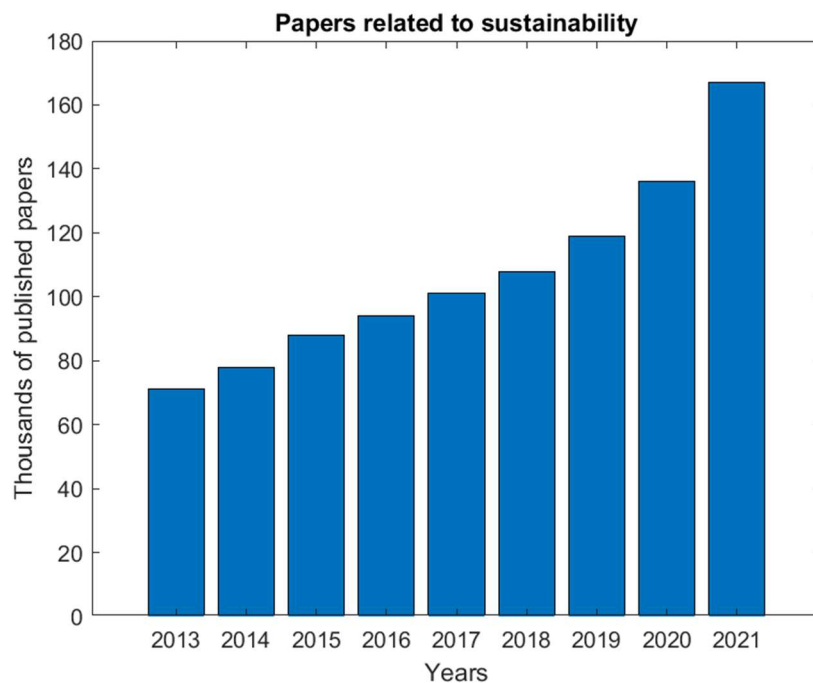


Figure 1. Papers related to sustainability. [2]

As Figure 1 confirms, interest for this topic is arising in all the scientific and social fields. In 2015, United Nations proposed the Sustainable Development's Goals (SDGs) to foster sustainable



Figure 2. UN Sustainable Development goals. [3]

development, including tackling environmental challenges and adopting cleaner production practices worldwide. [3] . This initiative sets seventeen goals that humanity should reach till 2030. The goals spaces from inequality reduction, cleaner energy, ecosystem preservation and many others. As shown in Figure 2, even if these goals are very different among each other, they have a point in common: in order to be reached, they need a smart management of economic, environmental and social resources.

These clear trend towards sustainability has started to influence many sectors, in particular those having the power to shift the market to other directions, as the finance and the economic fields. Forms of sustainable finance have grown rapidly in recent years, as a growing number of institutional investors and funds now incorporate various Environmental, Social and Governance (ESG) investing approaches [4]. Also, the awareness is growing on the causes of the environmental degradation we are facing. Many authors and agencies analyzed those issues, by attributing responsibilities to several industrial sectors, each of them characterized by different impact classes [5] [6]. In this context, due to the high number of players, causes of environmental degradation and impact classes, is important to carry on a detailed analysis, preventing the risk of simplified conclusions that may bring to wrong solutions.

In particular, the sustainability targets definition must rely on a detailed study of the interaction between the system that has to be “sustainable” and the effects that it causes, with a special focus for the negative impacts. Due to the techno-economic approach of this work a data-driven methodology for each measurable dimension of the sustainability will be preferred to a macroscale overview of the problems. Decomposition of the sustainability concept in all its derivation will be strongly related to the energy sector, identifying how this last is responsible for all the different impact classes. For each technological process is then necessary to track what are the interactions with the surrounding environment that may be a source of impact. This should lay the groundwork for the development of a sustainability metrics, which has to be as representative as possible of the peculiar situation it aims to analyze.

1.1 Sustainability in the energy context

The same general considerations developed in the previous section can be easily applied to the sustainability of energy systems. In general, an energy system is defined as a joint of technologies which aiming to produce one or more commodity. As the sustainability, also the energy system is a very wide concept. Its time and spatial scale may vary among several order of magnitudes. Also, the output commodities may change, spacing from simple electricity production to combined electricity & heat, or other energy commodities and sub-products, like hydrogen or ammonia as it happens in poly-generation systems. Since giving an overall overview of all the existing energy technologies would be difficult trying to include the extremely high number of options, a comprehensive definition is provided.

Also, this work must be restricted to a single category of energy systems, even if the general methodology could be applied (adapted) to all the existing systems. In particular, the following considerations will be applied to macroscale energy systems characterized by a long-time horizon and more than one technology involved. Concerning the output commodity, all the work will only refer to the sustainability of the electricity production. This choice is due to the consideration that power sector is expected to play a progressively larger role in the energy production mix in the next decades, with current energy strategies aiming at reducing GHG emission thanks to the electrification of end-uses and a higher renewables penetration in the electricity mix [7].

Many attempts have been conducted in defining sustainability in the context of macroscale energy systems, in particular for national and international applications of them. Two works represent the main contributors in this activity of defining sustainability in the energy context: the IAEA report

on energy indicators [8] and the WEC World Energy Trilemma Index [9]. A comparison between these two works may be beneficial, as proposed in Table 1.

In both the studies, the sustainability concept has been declined in its main dimensions (indicators), according to the different areas of impact at which the energy use is related. In turn, for each dimension one or more themes, which are still conceptual entities but more detailed, are individuated. For example, in the IAEA report [8] sustainability has been diversified in three main indicators but, in order to better define the problem, a set of seven themes and eighteen sub-themes is present. Taking as a reference the Environment indicator, the environment has been considered as the sum of atmosphere, water and land. For these last elements, sub-themes able to measure the direct impact of the energy use on them are inserted. Concerning the general approach, the methodology is similar in the WEC report [9], even if the considered voices are different.

Table 1. Comparison between IAEA [8] and WEC [9] sustainability evaluations.

IAEA			WEC		
Indicator	Theme	Sub-Theme	Indicator	Theme	Sub-Theme
Social	Equity	Accessibility	Energy Security	Security of supply and demand	Diversity of energy supply
		Affordability			Import independence
		Disparities		Resilience of the energy system	Diversity of electricity generation
	Health	Safety			Energy storage
Economic	Use and production patterns	Overall Use	Energy Equity	Energy Access	System stability
		Overall Productivity			Access to electricity
		Supply Efficiency			Access to clean cooking
		Production		Quality of Energy Access	Access to “modern” energy
		End Use			Electricity prices
		Diversification of Mix		Energy Affordability	Natural gas prices
	Security	Import			Gasoline and diesel prices
		Strategic Fuel Stocks			Affordability of electricity
Environment	Atmosphere	Climate Change	Environment	Resource Productivity	Final energy intensity
		Air Quality			Efficiency of generation
	Water	Water Quality		Decarbonization	GHG emissions from energy
		Soil Quality			Low carbon electricity generation
	Land	Forest		Emission and Pollution	CO2 intensity
		Solid Waste Generation			CO2 per capita
					CH4 emissions per ktoe
					PM2.5 mean annual exposure

From Table 1 it is possible to clarify why sustainability is considered a “wide concept”. Even if both the works aim at analyzing large scale energy systems, there is no accordance on which should be the set of sub-themes, not even in main ones. That is because, depending on the sensibility of each study towards a certain thematic, some aspects may be prioritized and others neglected. Nevertheless,

from this overview is possible to understand the main dimensions associated with the sustainability of the energy systems. Different layers of the energy problem can be highlighted by these two studies, as shown in Figure 3. Indeed, sustainability is a multi-layered bottom-up concept, because starting from the technologies which defines the energy system configuration, is possible to determine all the other aspects. Indeed, the choice of the technologies is at first instance responsible for all the above-mentioned aspects. Defining the technology mix of an energy system means defining its cost and the environmental impact that it will cause. Also, security and social aspects will be strictly related to the system configuration even if the dependence between them is less directly linked.

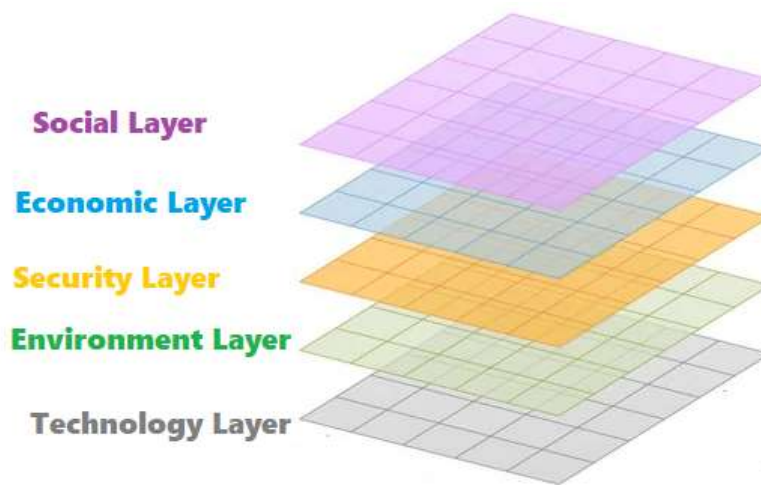


Figure 3. Different layers of the sustainability of the energy systems.

The various aspects of the sustainability problem in its interaction with the energy systems will be analyzed in the following.

The environment layer represents the interactions of the energy systems with the surroundings. Indeed, energy systems are responsible for different environmental impact classes as the consumption of resources (water, land, minerals...) and the emissions of pollutants and greenhouse gases. In order to establish the magnitude of those impacts is necessary to clarify the domain of the analysis. Indeed, impacts can be due to the only operational phase of the plants or to the entire life cycle. As mentioned before, the aim of this work is to leave the traditional “end of pipe” approach, moving to a holistic one, that’s why impacts have been accounted considering the whole life cycle of the plants.

In order to consider the life cycle environmental footprint of the energy systems needs a referenced and standardized methodology. At international level the LCA methodology is the well-established one and it is also ruled by the ISO 14040 series [10].

The life cycle assessment (LCA) approach aims at quantifying the environmental impacts of the complete life cycle of a general product [10]. Products can be intended as physical products, as goods to sell, but also as a commodity or a service, that is why is possible to apply it to the electricity production. As already said, the life cycle of a certain process is conned to a very high number of emission categories and use of resources such that the entire analysis will generate a huge set of parameters. Concerning the power production plants, LCA starts with the manufacturing all the plant to the dismissal of this last and, in parallel it covers all the impacts related to the fuel cycle. A better overview of the coverage of this approach is highlighted by Figure 4. Indeed, is possible to see the wideness of the LCA coverage, starting from the complete resource and energy requirements for the power plant, fuel extraction plant and fuel supply operations to the final decommissioning of them.

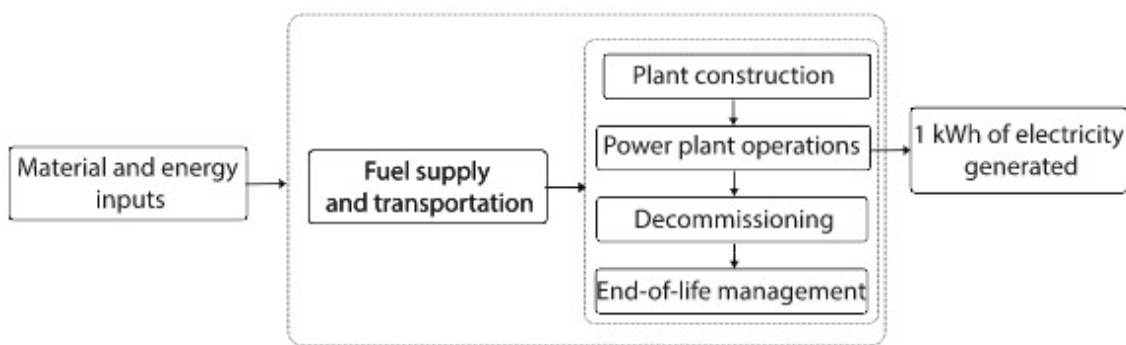


Figure 4. Life cycle stages covered by the LCA approach. [36]

Life cycle impact assessment (LCIA) helps the interpretation of LCA studies by translating the evaluated emissions and resources consumption into a limited number of environmental impact scores. This is done by means of characterization factors. Characterization factors indicate the environmental impact per unit of product (e.g., kWh of electricity per unit of resource used or emission released). There are two common ways of deriving these factors: at midpoint or endpoint. The difference between midpoint and endpoint factors is related to their location on the damage chain. Midpoint factors refers to the direct impact caused by the emission/consumption, for example the increase in GHG concentration caused by CO₂ emissions. Endpoint factors are instead located at the end of the chain and they can cover more areas. The two approaches are complementary in that the midpoint characterization has a stronger relation to the environmental flows and a relatively low uncertainty, while the endpoint characterization provides better information on the environmental relevance of the environmental flows, but it is also more uncertain than the midpoint characterization factors. For example, in Figure 6 there are four steps between the midpoint to the endpoint value of the damage, where each point introduces an error. An emission of a greenhouse gas (kg) will lead to

an increased atmospheric concentration of greenhouse gases (ppb) which, in turn, will increase the radiative forcing capacity (w/m^2), leading to an increase in the global mean temperature ($^{\circ}\text{C}$). Increased temperature ultimately results in damage to human health and ecosystems. [11].

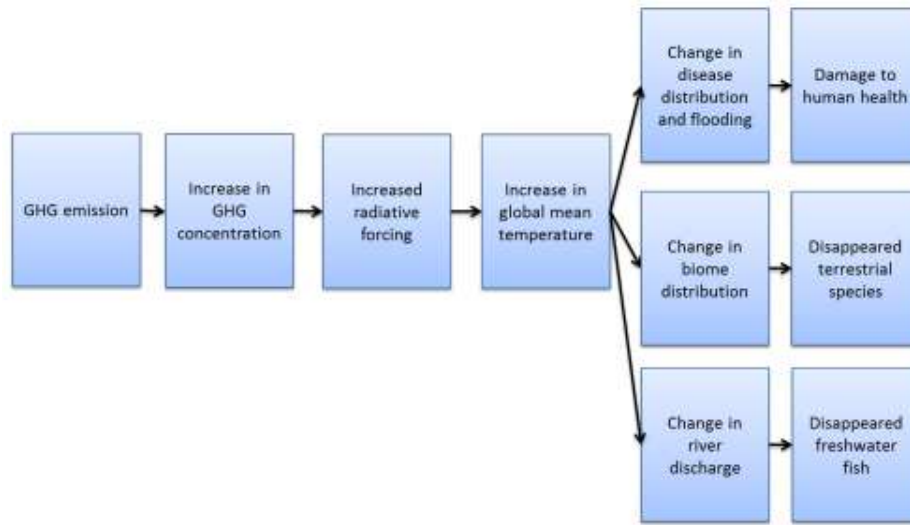


Figure 5. Cause-and-effect chain from greenhouse gas emissions to human health damage and relative loss of species in terrestrial and freshwater ecosystems.[11]

Proceeding to the next level of Figure 3, we found the security layer. Security means the system capacity to meet current and future energy demand reliably, withstand and bounce back swiftly from system shocks with minimal disruption to supplies [12]. The indicators cover both the management of internal and external energy sources, as well as the reliability and resilience of energy infrastructure. There are properties of an energy system which are intrinsically related to the technologies involved and other aspects related to the external situation. However, in order to compute a good security indicator, both these aspects must be taken into account. Parameters related to the internal configuration of the system are the diversification of the power source in the final electricity share, the rate of dispatchable power or the maturity level of the technologies involved. Beside those aspects, is important to consider how much the system depends on the import of energy from abroad and how this import is diversified. In the parameter selection it will be clear how all the above-mentioned parameters are combined.

Equity (or Social layer, with little differences between the WEC [9] and IAEA [8] classifications) is related to system ability to provide universal access to reliable, affordable, and abundant energy for domestic and commercial use ([8], [9]). This dimension captures basic access to electricity and clean cooking fuels and technologies, access to prosperity-enabling levels of energy consumption, and affordability of electricity, gas, and fuel. In general, the social layer related

indicators are all the parameter that capture a relation between the energy system and the well-being of the society that benefits of this system.

The economic layer is related to the overall cost of the energy system, but it can be interpreted in a different way depending on the player. A player (or an agent) may be a simple user, a company or a government. For each of these entities the economic problems related to energy will assume a different meaning. In order to better explain this sentence, some considerations are required: from an economic perspective, electricity consumers will be much more interested in the commodity price, which is a problem of affordability and accessibility that, as highlighted in Table 1, are both social and economic parameters. Governments and institutions may instead be focused on parameters like the total investment costs, the stock reserves or the import from abroad, aspects that fall under the security-economic problem [13].

1.2 How to measure sustainability

As mentioned in the previous section, sustainability is studied in all the economic, social and scientific fields but, in order to pass from a qualitative to a quantitative description of this concept is necessary to diversify and detail these fields. In particular, here sustainability refers to the reduction of negative impacts on environmental, social, safety and economic layers caused by the power sector.

As mentioned before, sustainability is such a time and space case-specific and depending on the interest of certain aspects with respect to others, the data necessary to define this wide variable could dramatically change. How to deal with this issue?

The final aim is to consider the process involving all the interactions that it has outside the system to which it belongs and to analyze simultaneously economic, environmental and safety aspects of the sustainability problem. This means to intend sustainability as a branched concept, which is the result of several components, also characterized by different magnitudes, and this rationale will constitute a key point in the next step of this analysis.

Another point needs to be discussed. Until now, the abovementioned aspects of the sustainability, as the economic, environmental or safety type, are conceptual elements. Being the aim to create a metric, and then a qualitative representation of the sustainability it is necessary to switch from economic, environmental and other kind of metrics to a unique score grouping them together.

The process of creating metrics or indices able to evaluate different aspects and rapidly describe the reality of a problem is a recent topic. It was in the early 1990s, and therefore recently, that the Organization for Economic Co-operation and Development (OECD), an intergovernmental organization of developed countries, conceived the purpose of using indicators as a tool for monitoring and disseminating information [14]. The favor met by the indicators strengthened the interest in them, up to the production of the OECD Report, which set the fundamental objective of giving the appropriate definition: "The indicator can be defined as a parameter, or a value derived from parameters, which provides information on a given phenomenon" [14]. The indicator has a meaning that goes beyond that of the single parameters from which it derives, as it has a synthetic meaning and is developed for a specific purpose.

Before getting into the core of the matter, it is important to highlight that indicator, index and parameter have different meanings:

- **Parameter:** A property that is measured or observed. Parameters are the primary data of each problem. In general, a parameter is a numerical entity characterized by its own metric. Examples of parameters are the GDP of a nation in economy or the CO₂ emissions for each Km of a car.
- **Indicator:** A value derived from one or more parameters which aim is to provide qualitative information about a certain phenomenon/dimension characterized by its parameters. Usually, an indicator is a dimensionless amount that should intuitively represent a degree of satisfaction with respect to a certain aspect. (e.g., a mark, a score...)
- **Index:** A set of aggregated indicators. Usually, an index is a dimensionless amount that should intuitively represent a degree of satisfaction with respect to all aspect complained by its indicators.

Here it comes an important convention that will drive the whole analysis. At least for the first part of the work, sustainability will be evaluated as an index. This convention is adopted to create a consistent evaluation scale for different technological processes that has as output the same unit of flow since this is the only way to guarantee comparability. Given that a concept as wide as the sustainability refers to several aspects, these aspects will be evaluated as indicators that, once combined, creates the final sustainability index.

Indeed, sustainability evaluation is a hierarchical process. Since sustainability is a composite concept related to several aspects, its final formulation should reflect this structure. In particular, sustainability will be a composite index, formed by several numerical indicators, where each indicator is referred to a particular aspect (or layer) of the sustainability (Economic, Security, Environment) [8]. Is important to highlight the difference between the sustainability, which is an index, and the several indicators. An indicator expresses a value related to a feature of a system, while with the term index we refer to a set of aggregated indicators. The step from indicators to index pass through a combination of the formers, which can be reached through a sum, an average or a different process. Both index and indicators provide a value which is qualitative. Indeed, they are scores that represent how the system well/badly behaves with a scale of figures. Qualitative evaluation must be performed relying on quantitative data. Indeed, indicators are derived from parameters that directly represent a certain phenomenon. For example, the environment indicator can be derived from parameters representing the emissions of pollutants of a certain system. Unlike the indicators, which are expressed by a qualitative score, each parameter is expressed in its own metrics. Combining different metrics will be an important task of this work.

An intuitive visualization is provided by Sanja et.al. [15] in Figure 6 where it is possible to highlight how the different parameters constitute indicators related to each of the sustainability aspects, and how these last are finally combined in the composite sustainability index. Before defining the different metrics inside each indicator is necessary to understand what aspects of the sustainability are more related to the energy systems topic.

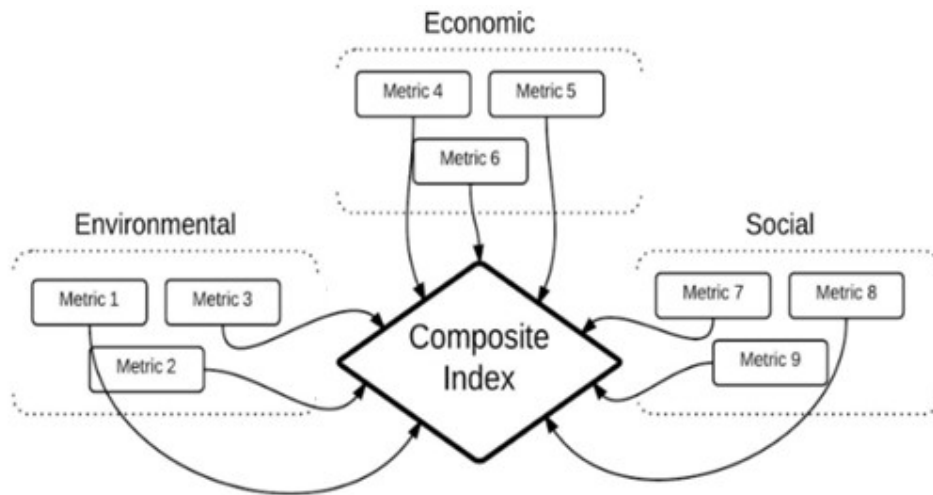


Figure 6. Sustainability composite index construction. [15]

Now it is easier to observe the complexities that the sustainability evaluation brings with itself and the high number of factors that must be taken into account, too. An important point to consider is about the combination of the sustainability indicators. The multidimensionality of the problem imposes the combination of different layers but, even inside the single layer different parameters must be considered. It must be remembered that the aim is to build a general score, defined in a specific metric, as the combination of all the layer scores.

There may be some interesting problems:

- Inside a single layer, two numerical parameters may have different relevance for the aspect at which they are related and, consequently, different weights should be used in the combination process of the parameters. For example, both affordability and accessibility belong to the security indicator, but the final value of the security indicator may be more related to the former aspect.

- Considering all the layers, some of them should need a higher weight in the final overall sustainability score of the analyzed scenario. Depending on the context for example, the environmental layer may have a higher importance with respect to the social one, and this must reflect into a higher contribution to the final sustainability score.

These two considerations make strongly necessary a calibration procedure of the sustainability score, because the relevance assigned to the different layers and, inside the single layer, to the parameters, plays a crucial role. In order to give a summary overview of the concept without entering in the details, let's take as an example the triangle visualization proposed by the World Energy Trilemma in Figure 7 [9]. In this specific case, for each aspect is defined a score which contributes of one-third to the final energy system evaluation.

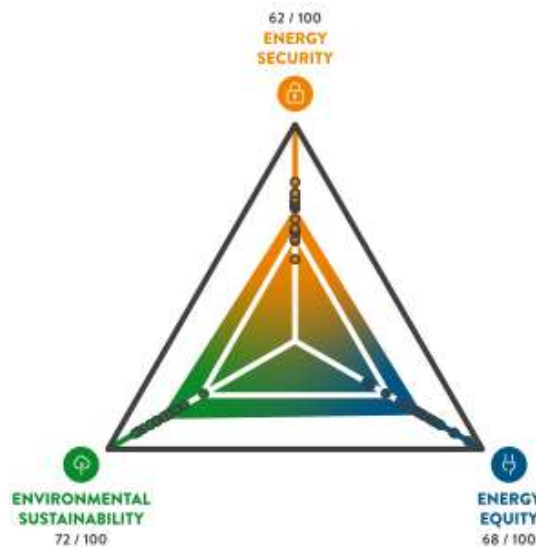


Figure 7. WEC Triangular Evaluation. [9]

What should arise from this general discussion is that there is not a unique way to account for sustainability in the energy related problems and, even if the indicators are defined, a discussion about how balance them is needed. As it happens in Figure 7, also in this work the issue of balancing parameters is solved thanks to a weighted sum approach, but this mathematical consideration will be treated in the following sections. The aim of this introduction is just to explain the problem from a conceptual point of view.

In conclusion, the sustainability assessment of an energy system requires several steps:

1. The identification of the different dimensions of the sustainability on which the energy system may have an impact, as the security, social and environmental ones.
2. The development of proper indicators for the considered dimensions, one indicator for each dimension. Indicator must be able to characterize, with a single numerical value, the behavior of the energy system with respect to its dimension.
3. For each indicator, the selection of proper parameters as comprehensive as possible about the dimension the indicator aims at represent. Parameters are, as previously explained, the primary data of the problem and each parameter is characterized by different metric.
4. The development of a framework able to give a qualitative evaluation (a score) for each indicator, starting from the parameters.
5. The development of a framework able to give a qualitative evaluation (a score) for the final sustainability index, combining together the different indicators.

These are the basic steps when performing an evaluation of an already existing energy systems for which all the data are already present. As anticipated in the abstract, aim of this work is to integrate the sustainability metric inside a bottom-up energy model, in order to let the final score to be accounted in the optimization algorithm. To better understand this second part, is necessary to clarify what energy models are, referring in particular to the bottom-up ones and also, why introducing sustainability considerations inside the model's paradigm is considered a reasonable and a necessary step.

1.3 Energy system optimization models and their limitations

The need to carry out medium / long-term planning at international, national or local scale, the growing attention paid to the reduction of greenhouse gas emissions, the optimal exploitation of resources, the economic impact of energy systems and the security of supply are some of the reasons that make the development of forecasting energy models important. Those models make it possible to analyze, over a long-term time horizon, the effects of various environmental and economic policies or possible technological evolutions on the energy system considered. Therefore, they aim to be tools not only used for scientific purposes, but also as support for decision makers.

The first step in creating an energy model is represented by the definition of the Reference Energy System (RES), that typically describes the entire technology chain, from energy supply to final service demands for each region. Extraction, primary and secondary production, import / export of energy and materials, processing plants and end-use sectors are represented in terms of processes (technologies) and commodity flows. Each technology (both existing and future) is described with economic (e.g., investment costs, operation and maintenance costs, etc.), technical (capacity factor, efficiency, etc.) and environmental (emission factors) parameters. As highlighted in Figure 3, RES constitutes the base-ground of the sustainability problem given that the technological configuration is the source of all the impacts in the other layers. An example of a simple regional reference energy system is shown in Figure 8.

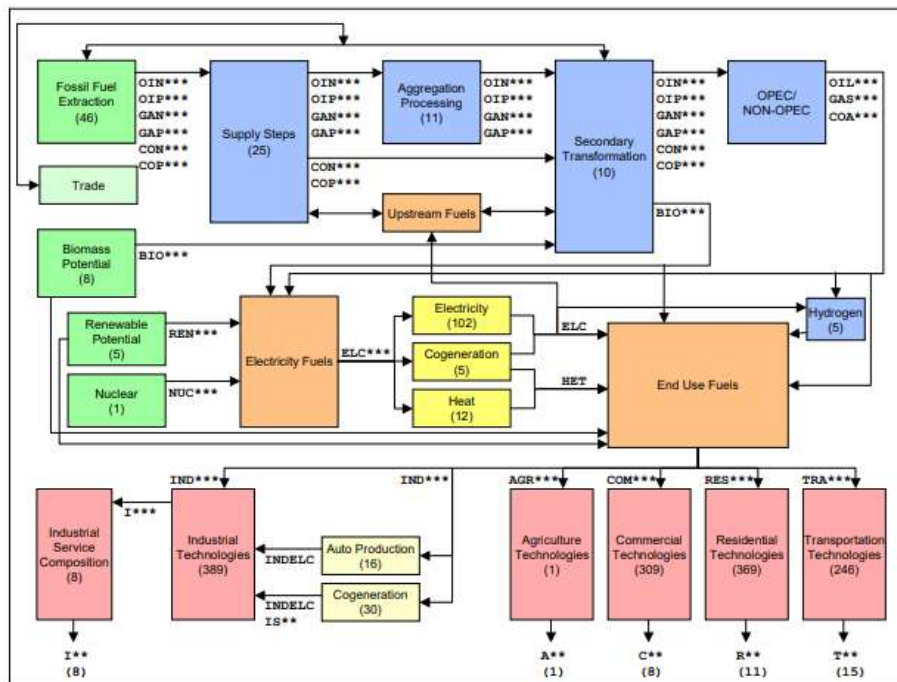


Figure 8. ETM Reference Energy System. [16]

Each attempt of analyzing an energy system aided by a calculator constitutes an energy model, for this reason a comprehensive classification of all the existing models will be too much detailed with respect to the aim of this section. For the purposes of this work, it is just necessary to enter in the details of the models used both in the ex-post analysis and in the endogenous integration of the sustainability paradigm.

Concerning the post-processing analysis whose aim is to test the sustainability score, the TIMES model generator has been chosen. According to its documentation, “TIMES (The Integrated MARKAL-EFOM System) is an economic model generator for local, national, multi-regional, or global energy systems, which provides a technology-rich basis for representing energy dynamics over a multi-period time horizon. It is usually applied to the analysis of the entire energy sector, but may also be applied to study single sectors such as the electricity and district heat sector” [16] [17]. All the models characterized by a technology-rich basis are called bottom-up models. Here it comes the first important definition.

Those models are used to analyze the dynamics of various energy sectors (e.g., energy, industry and agriculture), also taking into account the introduction of new technologies. Macroeconomic data are always exogenous and therefore such models are not able to evaluate the feedback effects on the economic system of technological developments. In these partial equilibrium models, the technologies of production, transformation and end use (existing and planned / possible) are described by technical (capacity, efficiency, life, availability factor, energy consumption, etc.) and economic (investment cost, fixed management and maintenance costs, variable costs, etc.). The optimization procedure allows to define, over the entire time horizon and with constraints and scenarios defined by the user, the overall mix of technologies (for the end-use sectors, for the production of electricity, etc.) and commodities (oil, natural gas, coal, etc.) which at the same time satisfies the demand for services and minimizes the total discounted cost of the system.

Bottom-up models are technology-oriented models. On the other side, top-down models are market-oriented models with an endogenous integration of the macroeconomic variables. Due to their market-oriented approach, they have limited representation of the energy sector and lack detail in the description of existing and future technologies, which are typically identified by aggregate production functions for each economic sector. Therefore, top-down models are useful in analyzing the evolution of energy prices and macro-economic variables but not for comparing the effects that different scenarios have in the selection of the best technologies.

As already mentioned, primary interest of this analysis is in the technology layer of the energy problem. That is why the choice of the models fall on the bottom-up type. The second important classification is between simulation and optimization models. Simulation models evaluate, in a parametric way, the response of a system to a given set of technical or political variables and identify the possible impacts and probable costs / benefits of the analyzed configuration. These models do not allow to find an optimal value for the aforementioned variables, but only allow to compare two or more scenarios. Optimization models calculate, for all the system variables, the values that lead to the optimal configuration, which is the configuration that minimizes / maximizes a given objective function (for example, an economic objective function coinciding with the total discounted cost of the system).

According to this classification, TIMES is a bottom-up optimization model. The optimization function of TIMES aims at maximizing is the total surplus, the economic situation that happens when price equals marginal value.

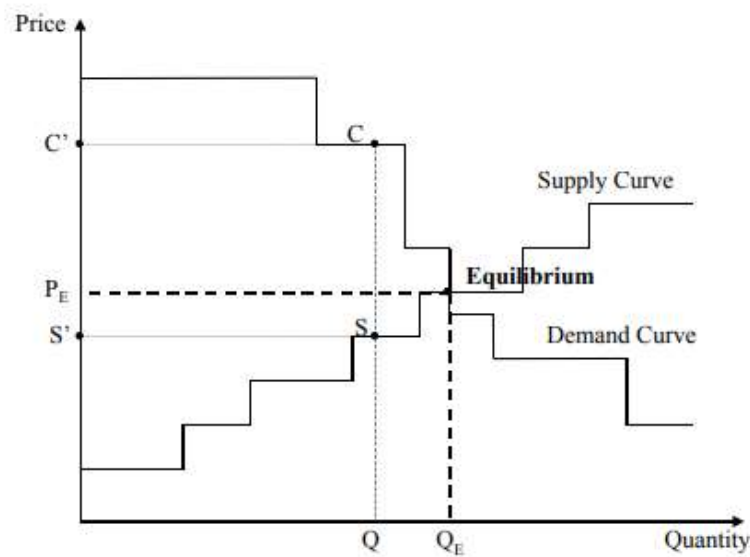


Figure 9. Equilibrium that maximizes the total surplus. [17]

As show in Figure 9, model aims at reaching the point in which supply and demand are balanced with the quantity and price vectors that maximizes the total net surplus of producers and consumers. As the quantity produced increases, one or more component the energy production mix (like a technological potential to produce or to a plan to extract) is exhausted, and therefore the system must start using a different (more expensive) technology or set of technologies in order to produce additional units of the commodity, increasing the marginal cost of the production. This concept is well explained by Figure 10.

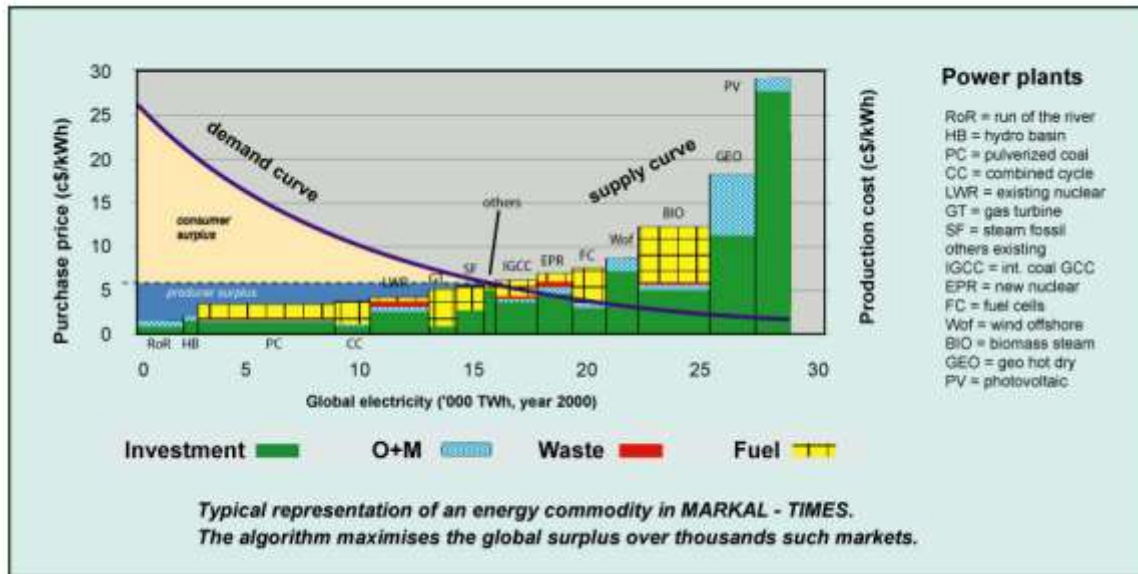


Figure 10. Schematic of the surplus maximization mechanism. [17]

In the last years, energy models have experienced an evolution in terms of numbers and in relation with the new applications and problematics that are arise. Objective of forecast models is to predict optimal technology configurations scenarios, in order to allow a comparison of the different alternatives. The main limitation is in the rationale behind the selection of the proper technology mix and, referring to the power sector, of the electricity production mix. The challenge of energy models in following the sharp electricity system revolution recently happened is still in progress. Nevertheless, is possible to identify at least two fronts in which a further evolution of the existing frameworks is needed. To better explain these problems, let us take again the TIMES model generator, in its most recent applications, as a reference.

In TIMES, the rationale behind the optimization algorithm is related to an economic principle. In particular, the terms of the objective function are costs that are proportional to the system operation. This is not necessarily a wrong, or monodirectional way of intending the energy problem. Costs may be a truthful indicator of all the energy related issues. For example, the external costs of energy related to a lack of supply can be internalized in the objective function of a model, and this may happen for

many other factors. So, there is no reason for excluding a priori an economic oriented objective function.

Many projects have been developed in this direction, also with TIMES. NEEDS project (New Energy Externalities Development for Sustainability) [18] has been the first attempt moving in this direction. NEEDS target was to evaluate the full costs (direct and indirect) of future energy systems. The goal was achieved by performing monetary evaluation of externalities associated to energy production, transport, conversion and use, creating an impact-cost database of all the energy technologies [18]. For each area of interest the external cost has been related to the production of a unit of electricity, creating something similar to a LCA database. The external costs of energy analysis was carried out by the ExternE project in 1995 [19] [19] which was the first systematic approach to the evaluation of external costs for a wide range of different electricity production systems.

Approach conducted by ExternE was, for the time, very innovative. Actual literature still relies on that framework [20] due to its peculiar methodology. To determine the final cost related to a certain impact, social cost (increasing of public health cost, death, loss of biodiversity) was related to the emissions of pollutants that cause the impact. Is a similar process to the calculation of endpoint LCA indicators. This approach, clearly explained by Figure 11, allows to create a connection between the activity of a plant and the monetary cost caused by a certain damage.

The advantage of this approach is allowing the direct accounting of some sustainability related parameters in the objective function, with the consequence of influencing the final electricity technology mix.

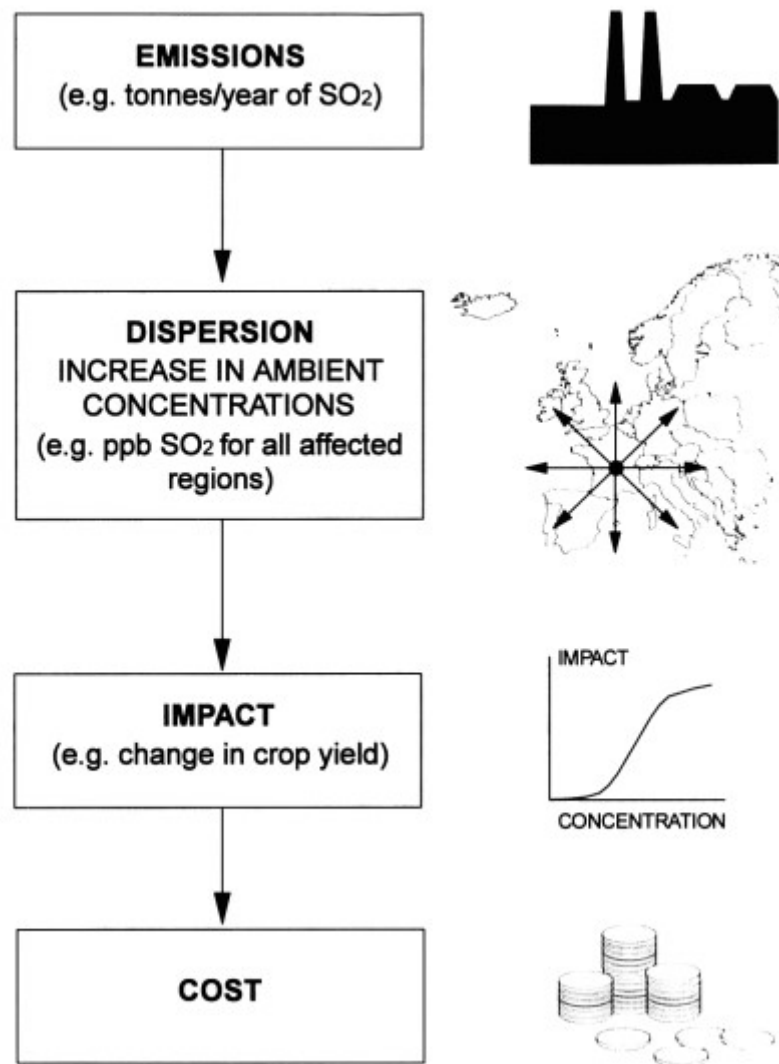


Figure 11. Steps of the damage accounting methodology applied to the consequences of pollutant emissions. [19].

Despite the innovation brought by ExternE, there are some problems that must be considered:

- There is a high uncertainty introduced by the monetization step, in particular, the damage-cost correlation is totally independent from the local environment.
- Focus is only on emissions related parameters. Other important aspects, like resource consumption, waste creation and energy security issues are unaccounted.
- Emission parameters follow, again, the old “end of pipe” approach. Life cycle emissions are neglected.

The aforementioned issues are mainly related to the ExternE methodology or to the impact assessment methods, but there are further limitations imposed by the TIMES modeling environment. In particular:

- The possibility of implementing different sustainability aspects, even if possible, needs an impact-cost approach. This means that all the sustainability layers (and the targets related to these last) must be translated in monetary units.
- Even if other cost voices can be integrated in TIMES, the model paradigm (intended as the objective function general formulation and the optimization algorithm) cannot be changed.
- Given that TIMES is a commercial tool modifying the abovementioned aspects is quite difficult.

These considerations automatically exclude all the parameters non translatable in monetary units, highlighting the necessity to find a different modeling environment.

The major issue that the TIMES model generator arises is the inaccessibility of the source code. Given that the second part of this work aims at changing the objective function of the model, integrating inside it a sustainability metric, an open-source framework is necessary. In this context, the use of a new modeling framework called Tools for Energy Model Optimization and Analysis (TEMOA) [21], could be beneficial for this analysis. In particular, an open-source model allows the direct modification of the objective function, the creation of new modules and the choice of a proper solution method (assigned to the model solver). These aspects are fundamental when moving in the direction of a high flexibility framework, due to the different implications that the sustainability problem may present. Indeed, TEMOA is formulated as a linear programming problem and is implemented in Python using Pyomo. Indeed, Pyomo is a Python-based open-source software package that supports a diverse set of optimization capabilities for formulating, solving, and analyzing optimization models [22]. An especially important feature of Pyomo is that it can be used to define general symbolic problems, create specific problem sets of expressions, and solve these sets using commercial and open-source solvers. The possibility of using different solvers will be extremely useful for this analysis.

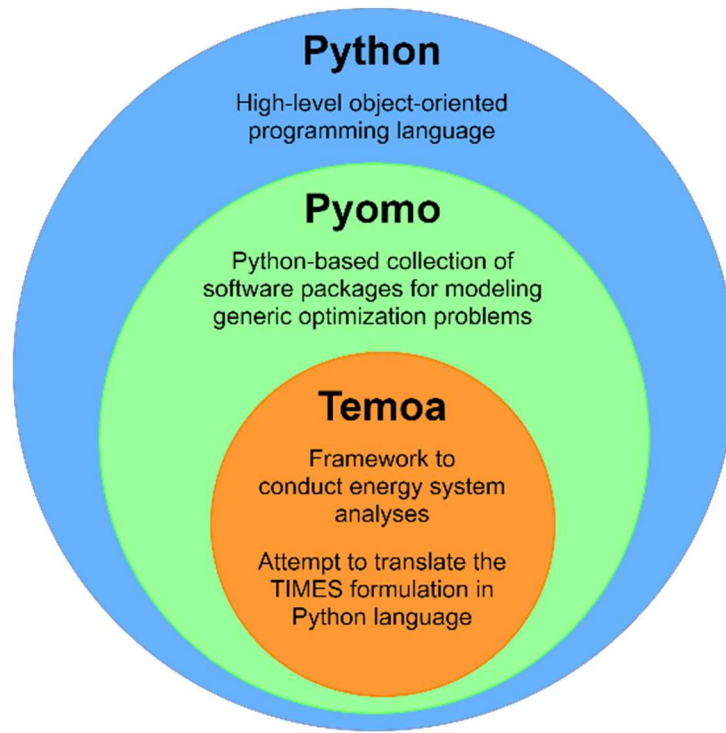


Figure 12. TEMOA framework based on Python-Pyomo integration. [21].

TEMOA model is a bottom-up, technology-explicit partial equilibrium energy system modeling framework devoted to energy system optimization. The formulation of the model is strongly influenced by TIMES model generators. The aim of the model is to minimize the present system-wide cost of energy supply by optimizing technology capacity and commodity flows to meet end use demands. The reason behind the choice of TEMOA rely on the need for open science and also, to the comparable performances with respect to TIMES, also proven by the comparison of the outcomes of the TEMOA-Italy and the TIMES-Italy model in [23].

1.4 Aim and structure of the work

After the wide explanation of all the interconnections between energy models and sustainability, is necessary to clarify in an exhaustive manner what in the previous section has just been mentioned, without entering deeply in the details.

The final objective of this work is the implementation in an open-source bottom-up energy modeling framework, the aforementioned TEMOA tool, of an optimization strategy able to account for both economic and sustainability aspects. Accounting for more than one aspect in an optimization framework falls under the area of multi-objective optimization problems.

Multiobjective optimization (MOO, also known as multicriteria optimization, multi attribute optimization, or Pareto optimization) is an area of multiple-criteria decision-making, concerning mathematical optimization problems involving more than one objective function to be optimized simultaneously [24]. Active part of this work will be devoted to the study of a proper solution technique which allows a decision-based objective algorithm. In particular, the sustainability and the economic components will be integrated in such a way that the final user is able to decide the relevance assigned at the components.

At the end, the model will fall on an optimized solution which should be the best compromise between the two objectives. Moreover, due to the very wide set of meaning that the sustainability concept may have in relation to the context in which it is applied, the final framework should be as flexible as possible. The strategy applied to reach this goal is composed of two steps:

Ex-post analysis, assess the impact of TIMES scenarios:

Known the time and spatial horizons of our problem, as explained before sustainability must be defined and declined in its relevant components. This means applying the sustainability concept at the local energy system under analysis, by looking for the fundamental aspects that characterize a sustainable energy scenario. These aspects will serve as components of the final composite index. The sustainability score is the resultant, obtained through a weighted average process, of the different sustainability layer indicators. At this point, indicators are conceptually, but not numerically, defined. Indeed, numerical indicators require a parametrization into quantitative values, creating a framework able to combine different metrics, again with a weighted average process. Finally, the developed sustainability index calculation procedure will be applied to several scenarios coming from the TIMES model generator, to validate the whole procedure.

A new optimization paradigm for sustainability assessment:

After having developed and tested the sustainability evaluation method in the post-processing phase, this framework should be integrated inside TEMOA. The final aim of the framework integration is the direct accounting of the sustainability score inside the objective function, by inserting it inside this last or as a model constraint. In the former method the weighted sum optimization method is used, while in the latter ϵ -method is necessary. Moreover, since the goal is to let the user to prioritize or penalize the economic or sustainability performances of the energy system, in the weighted sum approach weighting factors have been associated at the sustainability and economic components present inside the final objective function. The two model versions, differentiated by the multi-objective implementation strategy, are applied to a very simplified version of the TEMOA-Italy model, developed for test purposes. The purpose of this second part is not to provide useful outcomes for energy policymakers, but to test the new methodology developed in order to understand how a sustainability paradigm drives the evolution of energy scenarios.

Chapter 2: Ex-post analysis, assess the impact of TIMES scenarios

This section enters in the details of the post-processing sustainability assessment framework development.

The first part will be a review of the existing literature, many authors in recent publications debated about this topic and, in order to find a common path in this scientific work, a detailed analysis of the main works is necessary.

After that, Sustainability concept referred to the specific case of the Italian energy system is declined in its main indicators and related parameters. This delicate phase aim at the defining the structure of the sustainability framework calculation method and its dataset.

Then, it follows the mathematical part of this section. Sustainability parameters dataset is analyzed and elaborated, creating a procedure that allow to transform a defined set of different metrics into a single sustainability value. Framework is finally used to calculate the sustainability index of various TIMES-Italy scenarios. Results of this analysis are discussed with a view to the implementation inside the model phase that follows.

2.1 Review of the existing literature

A comprehensive overview of some important works about the topic, highlighting the main differences, is show in Table 2. In current existing literature, there are many approaches at the sustainability assessment of the power sector. In the analysis of different approaches, it is possible to find some trade-offs when trying to include different components in the sustainability concept. Choices must be made in sectorial coverage (only power sector [25], power and heat [26] , hydrogen [27]), time and spatial horizons (small scale plants, regional, national and international) but not only. In all the ex-post analysis considered there were also differences among the selection of the life cycle stages and the number of other aspects considered. Some studies are more related to the environmental aspects of the sustainability [22], while others to the energy security and the infrastructure requirement. Furthermore, there are studies that adds a dynamic component to the LCA parameters [25], by making these lasts vary with the technological improvement. This procedure will be better explained in the analytical part and is called Harmonization.

Differences are present also in the methodologies. Some papers rely on a simple ex-post approach that analyze separately each impact [28] , while other works perform a deep Multi Criteria Decision Analysis [29]. The characteristics of the former approach are the capability to deal with real quantities for all the analysis, but at the same time there is a limitation on the parameter that can be considered. Indeed, in a simple ex-post analysis there is no possibility to account together for different aspects. Instead, in a MCDA process, at a certain point of the analysis is necessary to pass from parameters, with their own metrics and related to a certain sustainability aspect (pollutant emission, energy affordability, etc.), to a numerical score, but the advantage is to consider together different aspects.

A final note is made on the use of energy models in this section. Since the post-processing phase only requires future energy scenarios, independently on the way these last has been generated, there is no focus on the model used in order to get the outcomes. Nevertheless, TIMES has been used in most of the papers ([24],[27],[28],[30],[31]).

As it can be appreciated, differences among the selected works are mainly related to the space and time domain and in the methodological framework. If interested in creating a flexible tool, the former aspect is not relevant. It could be interesting to analyze the three different approaches: Ex-Post, MCDA and the THEMIS framework.

Table 2. Main literature about the sustainability assessment of the power sector trough energy models.

Study Feature	[25]	[28]	[30]	[31]	[32]	[33]	[29]
Sectorial coverage	All	Power sector	Power sector	Power sector	Power sector	Power sector	Power sector
Time horizon	2050	2050	2050	2050	2050	2050	2050
Space horizon	EU	EU	US	UK	UK	EU	Spain
Approach	Ex-Post	THEMIS	Ex-post	THEMIS	Ex-post	Ex-post	MCDA
LCA Stages	All	All	All	All	All	Partial	All
Harmonization	Yes	Yes	Partial	Yes	No	No	No
Open access	No	Yes	No	Yes	Yes	Yes	No
Technology description	Rich	Poor	Rich	Rich	Rich	Poor	Rich
Parameter description	Rich	Very Rich	Poor	Rich	Rich	Rich	Poor

For the Ex-Post analysis, the most complete work is the one conducted by Blanco et.al [25], about the integration of Life Cycle parameters with European TIMES scenarios. Figure 13 shows the two main elements of this study: TIMES model generator and LCA inventory. TIMES scenarios have been used to obtain the activity of primary and secondary processes. Several European policies has been simulated and outcomes of these scenarios has been mixed with LCA inventory data to provide the final impact for each category.

The information used from TIMES reference energy system for the LCA are mainly related to using efficiency, lifetime and capacity factors used to modify the original inventory from the databases. LCA data are reduced depending on the technological improvement and this procedure is called Harmonization.

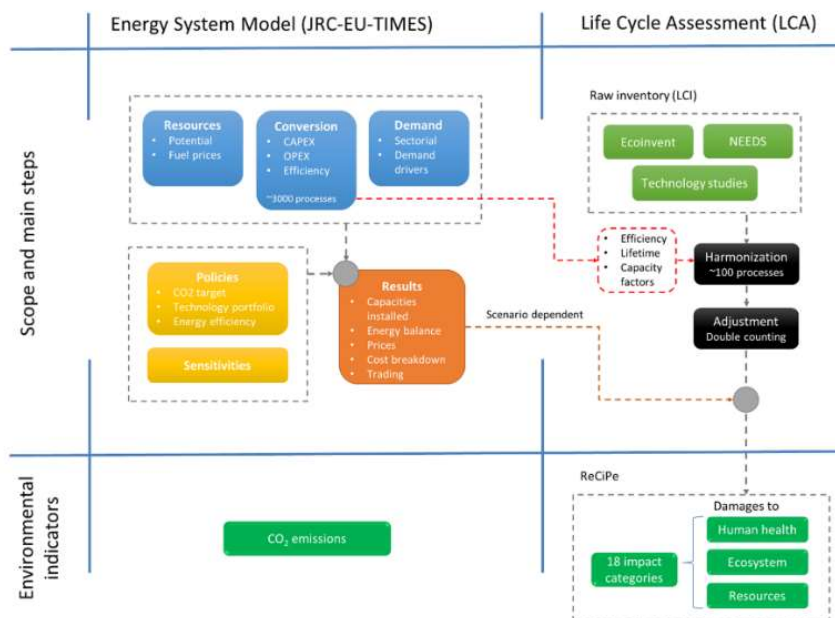


Figure 13. Framework for integrating LCA and energy modeling followed by Blanco et al. [25]

This approach is similar to the THEMIS framework presented by Gibon et al. ([28]). From its definition, THEMIS is used to evaluate technologies from a life cycle perspective by calculating the material and energy inputs and outputs to production, operation and maintenance, and disposal. The rationale behind the THEMIS account of impact is that, due to the increasing utilization of renewable energy technologies and energy conservation, the importance of quantifying life cycle impacts increases, as relatively fewer impacts take place directly at power stations and relatively more impacts occur upstream in supply chains.

Both THEMIS and the Figure 13 frameworks finally produce an evaluation of different scenarios divided by impact classes, in these cases, focused on the environmental layer of the sustainability.

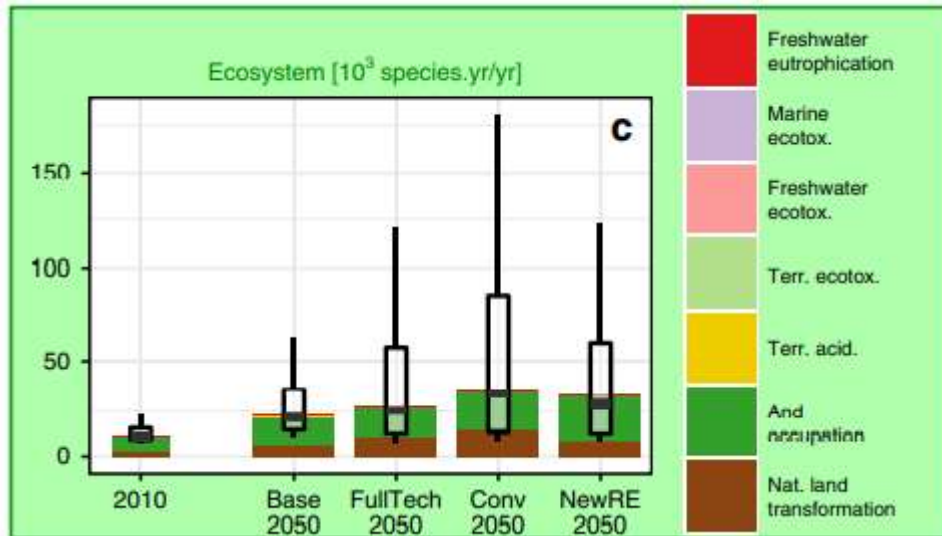


Figure 14. THEMIS Ecosystem evaluation of different EU policies scenarios. [28]

As shown in Figure 14 these kinds of tools are very useful in a post-processing context, when different scenarios has to be evaluated on the same parameter or, as it happen here, around a set of parameters for which the sum is allowed thanks to a common scale. In this case the common scale is guaranteed by the application of a Life cycle impact assessment (LCIA) calculation method at the single parameters (e.g Terr. Ecotoxic, Nat. land transformation) . The LCIA methods are extremely useful tools when interested in just one impact or, in general, a single aspect of the sustainability.

When interested in combining several aspects related to the sustainability of an energy system, advanced techniques as the Multi Criteria Decision Analysis are needed. In 2017, Gamboa et al. [34] proposed a very comprehensive review of almost all the existing MCDA works related to energy systems models. More than sixty papers have been analyzed, all related to the power sector and focused on sustainability aspects: Technical, economic, environmental and social. Aim of their publication, which has point in common with the aim of this work, was to evaluate different scenarios with a single value and they concluded that: “The use of an MCDA method becomes necessary and convenient to robustly prioritize the different energy scenarios according to the multiple evaluated criteria. In other words, the use of MCDA facilitates ranking energy scenarios by quantitatively addressing trade- offs between the selected criteria”. In other words, when dealing with single scenario sustainability indicators, the rationale behind the MCDA is necessary.

In conclusion, in order to make the first part of this work (and consequently the second) able to bring a positive contribution in the scientific literature a competitive advantage with respect to the other publications must be present. This is achieved by:

- Using as a technology layer a well-known and validated energy model generator, such as the TIMES one.
- Involving in the sustainability analysis both environmental parameters, coming from the LCA world and elaborated through a referenced LCIA method, and non-LCA parameters, related to the energy security and social layers.
- Make use of the harmonization procedure to add a dynamic component to the developed framework
- Involve the MCDA procedure in the mathematics formulation of the framework to achieve the scenario single score evaluation.

2.2 The TIMES-Italy power sector and the scenarios

Since the aim of the analysis is to apply the sustainability assessment framework at the TIMES-Italy power sector, it is necessary to define the reference energy system technologies at which the several parameters will be applied. In particular, the impact database will be associated at the activity of the power sector, or better, at the output commodity produced (in this case, only the electricity) and this kind of data is known for each scenario once it has been simulated. The mathematical correlation between the activity of the plant (expressed in MWh of produced commodity) and the different impact parameters is explained in the section devoted to the mathematical definition of the framework. For the moment, purpose of this part is to define the technological layer at which the impact parameters will be applied, without entering in the details of how this data will be used.

Two kinds of data are necessary: the power sector data and the activity for the different power plants for each scenario. Concerning the first type, these data are useful since we want to perform the harmonization of the LCA parameters then, we need to reduce the impact value by following the technological improvement. The driver selected for the technological improvement are: the capacity factor, the efficiency and the lifetime.

In Table 3 the TIMES-Italy power sector characterization in which is possible to find the abovementioned data is illustrated. Twenty-seven technologies are considered and for them technical data (Efficiency, Lifetime, Availability Factor) and economic ones (Fixed and Variable costs, Investment cost) are described.

Table 3. TIMES-Italy power sector technologies.

Technology Description	Efficiency	Lifetime	Investment cost [€/KW]	Fixed operation and maintenance cost [M€/KW]	Variable operation and maintenance cost [M€/GJ]	Availability factor
Gas turbine < 80 MW with steam	0.350	25	277	8.5	0.75	0.950
Gas turbine < 300 MW	0.336	25	160	8.5	0.56	0.950
Combined cycle (gas turbine-2006) < 3000 MW - AAT	0.530	30	550	12.3	0.56	0.900
CYCLE with steam turbine USC (2006) >500 MW coal - AAT	0.440	35	1200	22.0	0.31	0.760
Steam turbine USC-FGD (2006) < 2500 MW oil comb - AAT	0.432	40	969	18.3	0.31	0.850
Wind farm type A	1.000	15	1700	35.0	0.00	0.253
Wind farm type B	1.000	15	1700	35.0	0.00	0.213
Wind farm type C	1.000	15	1700	61.0	0.00	0.253
Wind farm type D	1.000	15	1700	61.0	0.00	0.213
Off-shore wind farm	1.000	20	4000	60.0	0.00	0.427
Off-shore deep water wind farm	1.000	20	2740	75.0	0.00	0.540
Bioliquids plant	0.310	15	2350	75.0	1.11	0.700
Biomass plant 5 cEuro - AT	0.255	15	2350	75.0	1.11	0.571
Biomass plant 12 cEuro - AT	0.255	15	2350	75.0	1.11	0.571
Biomass plant 5 cEuro - AAT	0.350	20	475	60.0	1.11	0.760
Biomass plant 12 cEuro - AAT	0.350	20	475	60.0	1.11	0.760
Mini hydro	1.000	30	4500	78.0	0.00	0.534
Mini hydro >1 MW	1.000	30	2250	33.0	0.00	0.534
Geothermal plant - AT	0.100	15	4000	86.0	0.00	0.856
Geothermal plant - geocycles	0.100	15	6000	86.0	0.00	0.880
PV roof plant	1.000	20	5000	45.0	0.00	0.306
PV ground plant	1.000	20	4350	43.5	0.00	0.306
Biogas Agro-Zoo - BT	0.320	9	3500	75.0	0.00	0.580
Biogas Waste - MT	0.320	9	1100	40.0	3.19	0.485
Solar with storage	1.000	25	5500	70.0	0.05	0.700
PEM fuel cell system running on hydrogen 100 kW based	0.450	15	3000	37.5	29.17	0.900

Together with the power sector, it is important to define the electricity generation scenarios on which the postprocessing analysis is conducted. Three scenarios are used to test the framework, with an increasing degree of decarbonization: Business-as-usual, Moderate and Aggressive. These three scenarios are characterized by different growth rates for renewables and fossil fuels power plants. In particular, for renewable power plants growth rates are positive and for fossil ones they are negative. According to the intensity of decarbonization (moderate or aggressive) growth rates are increased. For the business as usual scenario in Figure 15, the electricity production mix has been kept almost constant.

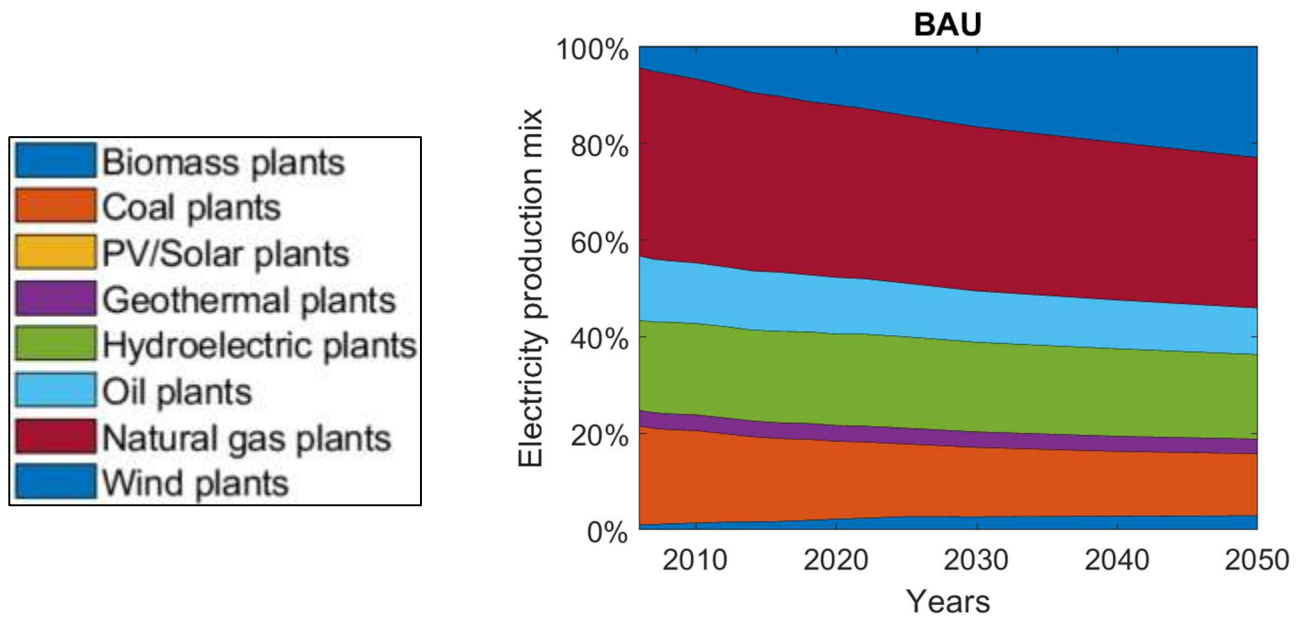


Figure 15. Business as usual TIMES-Italy scenario.

As it can be appreciated by Figure 15 this scenario is mainly composed of fossil fuels power plants such as gas, coal and oil. Here the target is not to decrease the emissions but just to preserve the energy mix constant through the years. A business-as-usual scenario is helpful for the analysis since it allows to appreciate the differences with respect to low carbon evolutions of the energy system. For all the figures related to the different scenarios only the electricity production share is plotted. The rationale behind this choice is related to the framework formulation that will be explained in the next sections. Indeed, in the methodological part it will be clear that the interest is localized in the technological evolution of the system that, ultimately, determines the sustainability value of the scenario. So, the focus is on how the electricity is produced instead of the overall amount produced.

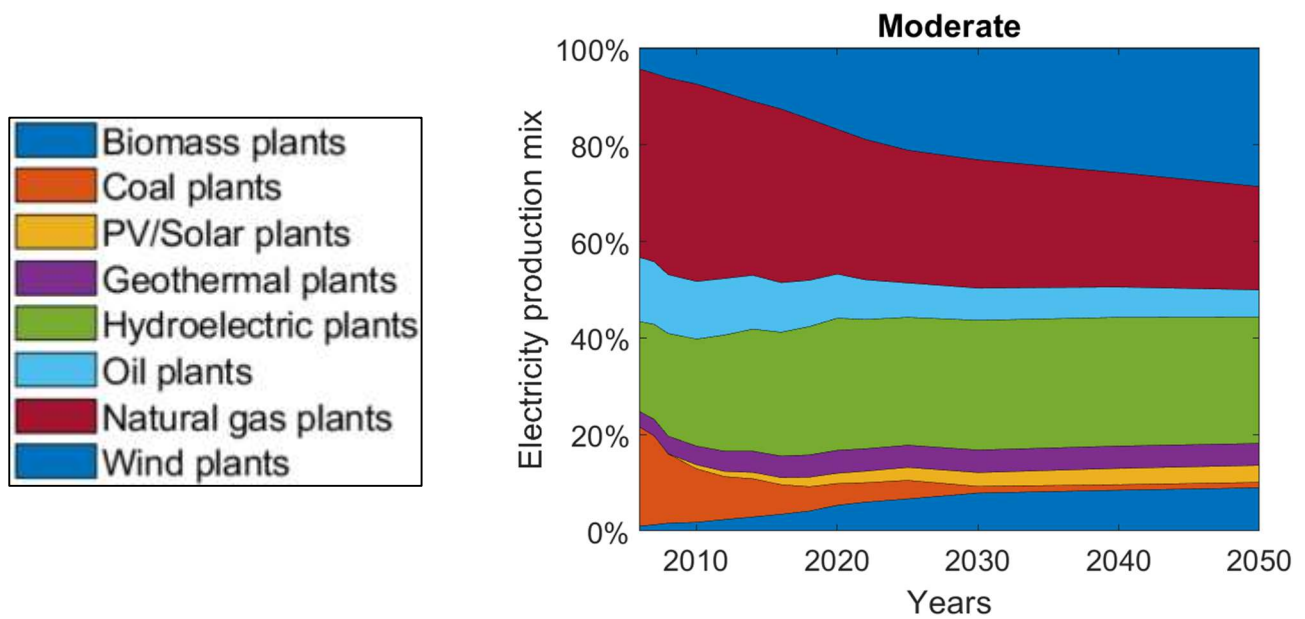


Figure 16. Moderate TIMES-Italy scenario.

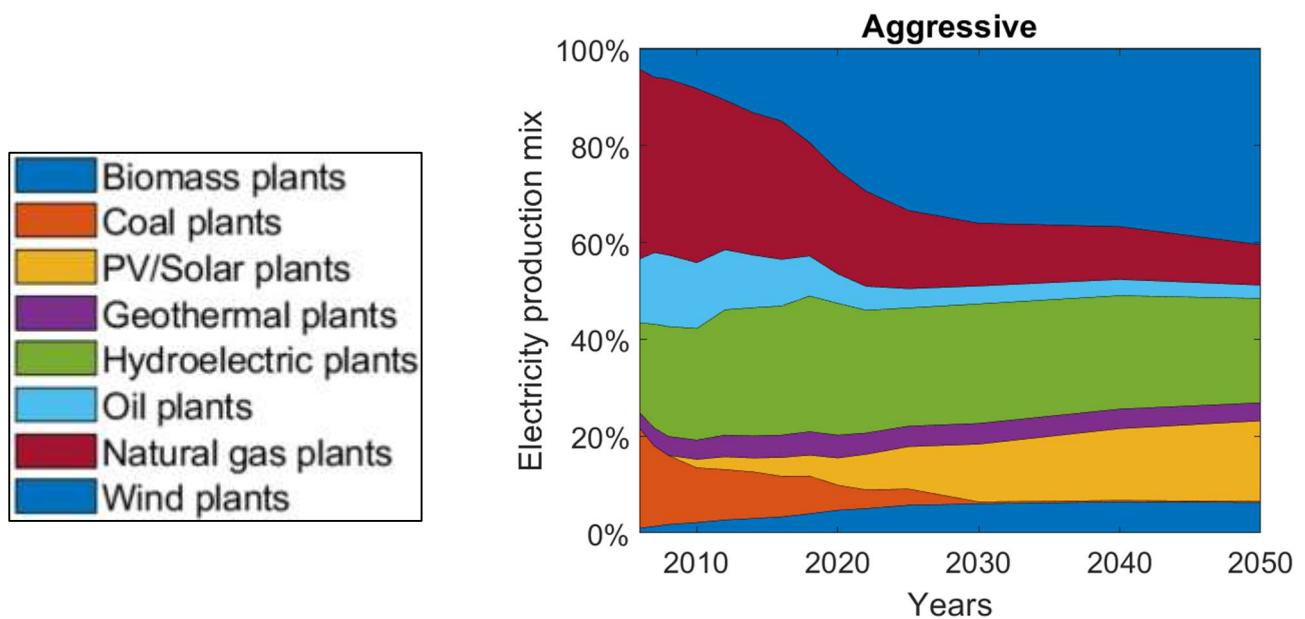


Figure 17. Aggressive TIMES-Italy scenario.

In Figure 16 and Figure 17 is possible to appreciate the other two scenarios on which the framework is applied. Is clear from the pictures that the decarbonization target is higher. There is a phase out of the coal power plants with a tangible reduction also of oil and gas use for power generation.

2.3 Indicators and parameter selection

According to the World Energy Council [8] and the International Atomic Energy Agency [8] and the comparison made in Table 1 these are the main aspects individuated that may serve as indicators:

- Economic
- Environment
- Equity (or Social)
- Security

The target of the metric is to be as comprehensive as possible, but also concrete. That is why aspects too far from the technical energy discussion will be neglected. For example, energy related problems like the increase/decrease of occupation in the energy sector has been omitted not because it is considered irrelevant, but due to the difficulty in finding a direct correlation. Indeed, the social (or equity, from now these two terms may be interchanged) layer is mainly focused on the direct impact of the energy system, like energy price and human health parameters.

Concerning the economic aspect, there is an important consideration before introducing it as a sustainability indicator. In particular, there are economic aspects that can fall inside the other energy dimension, like the electricity price in the social layer. But, when considering a separated economic dimension, is necessary to remember that scenarios already come from an economic optimization. Moreover, the optimization aims at maximizing the total surplus, which is the sum of the seller and buyer components. For this reason, integrating an economic dimension in the sustainability metric will cause a sort of “double counting”. In conclusion, economic dimension has been avoided given that is already accounted in the optimization algorithm of the model to which this metric aims to be implemented.

Environmental indicator

The impact assessment of the environmental footprint caused by the energy system is one of the main reasons for which this analysis is started. Indeed, due to the higher penetration of renewables, environmental impact of the energy system has been shifted from the operational phase to the other parts of the life cycle of the plant. Moreover, actual models account for emissions (such as CH₄, NO_x and CO₂) without directly relating the emission value at the environmental impacts at which is associated. This direct accounting of the impacts is allowed only by the use of LCA databases connected to a proper life cycle impact assessment method.

In order to properly select which are the area of interest of the environmental dimension, a focus is given to the three main components of the environment: atmosphere, land and water. This is a very smart choice of the dimensions because life cycle impacts of plants usually act on different environment dimensions in different life cycle phases. For example, a coal plant can mainly impact the atmosphere during its operation but requiring a large water consumption and soil exploitation in the coal extraction phase. Also, in order to open a window at the relevant theme of material waste and recycling, strictly related with the actual circular economy topic, a parameter related to the waste creation has been selected.

Atmosphere related parameters

According to the parameters available with the ReCiPe LCIA method [35], damage caused by emission of pollutant in atmosphere can be accounted thanks to a ReCiPe already developed endpoint indicator or, by several midpoint indicators. Since the step from midpoints to endpoints parameters introduces errors, the following midpoint parameters are used:

- Global warming potential [KgCO₂eq./MWh]:

This parameter aims to quantify the Global Warming Potential (GWP) contributions of a plant along its life cycle from the ‘cradle’ – the extraction of the raw materials that are used construction the building - through to the ‘grave’ – the deconstruction of the building and how to deal with its building materials (recovery, reuse, recycling and waste management). The evaluation method relies in the accounting of all the GHG emissions, by multiplying them for their specific equivalence factor. This allows to pass from plant emission [GHG-type-Kg/MWh] to the activity related parameter [35].

- Acidification Potential [gSO₂eq./MWh]:

Acidification potential refers to the compounds that are responsible of acid rains. These include sulfur dioxide (SO₂), nitrogen oxides (NO_x), nitrogen monoxide (NO), nitrogen dioxide (N₂O), and other various substances. Acidification potential is usually characterized by SO₂-equivalence emitted for each MWh of electricity produced. Indeed, these acid gases are usually released into the atmosphere because of fuel combustion. Newly constructed power plants have a desulfurization technique to limit the SO₂ emissions to the environment. [35]

- Eutrophication Potential [gPO₄eq./MWh]:

EP is the EI responsible for the enrichment of nutrients in soil or water. This enrichment can be due to nitrogen and phosphorus from polluting emissions, wastewater, and fertilizers, originating excessive development of algae and plants. In water, this excessive development of microorganisms decreases the rates of oxygen and solar energy, leading to the contamination of plants and groundwater in terrestrial eutrophication. [35]. This parameter, again related to power plant emissions, has been selected in order to give at the atmosphere module a Water-Land direction.

In the next page, it follows Table 4 with the above-mentioned parameters defined for each TIMES-Italy technology.

Table 4. Atmospheric related LCA parameters for TIMES-Italy.

Technology Description	GWP [KgCO ₂ eq/MWh]	AP [gSO ₂ eq/MWh]	EP [gPO ₄ eq/MWh]
CYCLE with steam turbine USC (2006) >500 MW coal - AAT	970.00	430.00	129.00
Steam turbine USC-FGD (2006) < 2500 MW oil comb - AAT	970.00	430.00	129.00
Gas turbine < 80 MW with steam	787.00	967.00	110.00
Gas turbine < 300 MW	787.00	967.00	110.00
Combined cycle (gas turbine-2006) < 3000 MW - AAT	787.00	967.00	110.00
Biogas Agro-Zoo - BT	213.71	853.00	138.00
Biogas Waste - MT	202.87	853.00	138.00
Bioliquids plant	202.87	853.00	138.00
Biomass plant 5 cEuro - AT	384.38	853.00	138.00
Biomass plant 12 cEuro - AT	384.38	853.00	138.00
Biomass plant 5 cEuro - AAT	384.38	853.00	138.00
Biomass plant 12 cEuro - AAT	384.38	853.00	138.00
Solar with storage	104.00	528.00	44.00
PV roof plant	104.00	528.00	44.00
PV ground plant	104.00	528.00	44.00
Wind farm type A	11.00	61.00	4.00
Wind farm type B	11.00	61.00	4.00
Wind farm type C	11.00	61.00	4.00
Wind farm type D	11.00	61.00	4.00
Off-shore wind farm	9.00	50.00	2.70
Off-shore deep water wind farm	9.00	50.00	2.70
Mini hydro	4.00	0.00	0.00
Mini hydro >1 MW	4.00	0.00	0.00
Geothermal plant - AT	41.00	190.00	24.80
Geothermal plant - geocycles	41.00	190.00	24.80

Water and Land use parameters

Complete dataset for Water and Land use were not present in the NEEDS Database. These two parameters are taken by existing literature about the topic. In particular, Land Use data are taken from International Renewable Energy National Agency (IRENA) Global Land Outlook [36] [36] and Water Use from National Renewable Energy Laboratory (NREL) report [37] [37].

Concerning the water is necessary to specify the difference between parameters easily available on literature. In particular, water withdrawal refers to water removed for the source for use, while water consumed refers to water used and evaporated, so that this last is not available at the same location. Data are referred to the second type.

Table 5. Water Use and Land Use LCA data for TIMES-Italy.

Technology Description	Land Use [m ² /MWh]	Water Use [m ³ /MWh]
CYCLE with steam turbine USC (2006) >500 MW coal - AAT	0.30	1.94
Steam turbine USC-FGD (2006) < 2500 MW oil comb - AAT	0.30	1.94
Gas turbine < 80 MW with steam	0.20	0.91
Gas turbine < 300 MW	0.20	0.91
Combined cycle (gas turbine-2006) < 3000 MW - AAT	0.20	0.91
Biogas Agro-Zoo - BT	0.10	1.48
Biogas Waste - MT	0.10	1.48
Bioliqids plant	0.10	1.48
Biomass plant 5 cEuro - AT	0.10	1.48
Biomass plant 12 cEuro - AT	0.10	1.48
Biomass plant 5 cEuro - AAT	0.10	1.48
Biomass plant 12 cEuro - AAT	0.10	1.48
Solar with storage	10.00	0.34
PV roof plant	10.00	0.34
PV ground plant	10.00	0.34
Wind farm type A	1.00	0.08
Wind farm type B	1.00	0.08
Follows on next page		

Wind farm type C	1.00	0.08
Wind farm type D	1.00	0.08
Off-shore wind farm	1.00	0.08
Off-shore deep water wind farm	1.00	0.08
Mini hydro	10.00	17.00
Mini hydro >1 MW	10.00	17.00
Geothermal plant - AT	2.50	1.38
Geothermal plant - geocycles	2.50	1.38

Non-LCA environmental parameters

To complete the environmental module of this metric other parameters are needed. Waste creation and noise pollution has been considered. To relate the environmental aspect with a numerical indicator, considering that there are no free available databases which gives these data, assumptions are made. For the waste creation parameter, it has been assumed that the amount of waste material and the difficulties brought by the waste disposal and recycling are proportional to the decommissioning cost of the power plant.

Considering the noise pollution, data are obtained thanks to the noise level contained in the environmental declarations of several plants (one for each type considered in the model) available at the Italian Ministry For Ecological Transition [38]. The nature of this data is very different from the other. Indeed, these lasts are not related to the activity of the plant, and this may cause confusion. In the mathematical description of the framework, this aspect will be clarified.

In the next page Table 6 follows, where data for each technology are presented.

Table 6. Non-LCA environmental parameters for TIMES-Italy.

Technology Description	Noise Pollution dB(A)	Waste Creation Dec. Cost [t€/MW]
CYCLE with steam turbine USC (2006) >500 MW coal - AAT	117.00	90.00
Steam turbine USC-FGD (2006) < 2500 MW oil comb - AAT	117.00	90.00
Gas turbine < 80 MW with steam	46.00	100.00
Gas turbine < 300 MW	46.00	100.00
Combined cycle (gas turbine-2006) < 3000 MW - AAT	46.00	100.00
Biogas Agro-Zoo - BT	54.00	100.00
Biogas Waste - MT	54.00	100.00
Bioliquids plant	54.00	100.00
Biomass plant 5 cEuro - AT	54.00	100.00
Biomass plant 12 cEuro - AT	54.00	100.00
Biomass plant 5 cEuro - AAT	54.00	100.00
Biomass plant 12 cEuro - AAT	54.00	100.00
Solar with storage	57.00	0.00
PV roof plant	57.00	60.00
PV ground plant	57.00	60.00
Wind farm type A	51.00	105.00
Wind farm type B	51.00	105.00
Wind farm type C	51.00	105.00
Wind farm type D	51.00	105.00
Off-shore wind farm	212.00	0.00
Off-shore deep water wind farm	212.00	0.00
Mini hydro	290.00	97.00
Mini hydro >1 MW	290.00	97.00
Geothermal plant - AT	54.00	90.00
Geothermal plant - geocycles	54.00	90.00

Energy security parameters

The IEA defines energy security as the uninterrupted availability of energy sources at an affordable price [39]. Energy security has many aspects: long-term energy security deals with timely investments to supply energy in line with economic developments and environmental needs. On the other hand, short-term energy security focuses on the ability of the energy system to react promptly to sudden changes in the supply-demand balance. Is possible to claim that energy security is composed by two factors, a first one related to the security of the supply and a second more linked to the intrinsic security of an electric system.

Moreover, there is a limitation on the choice of the security data. Indeed, the selected parameters should be defined for each technology and, more important, known a priori. This means that parameters that translate into a numerical value the abroad dependence must be defined before running the scenario, and this is a big challenge.

Considering all these aspects, it follows a list of the selected parameters.

- *Abundance [Years of proven resource for a power plant fuel]:*

This parameter aims at quantifying the future resources of a certain fuel associated to the power plant at which the indicator is related. All the power plants with the same input fuel presents the same value for this parameter. Is a good indicator of how a certain plant is unreliable from the point of view of a possible scarcity of fuel.

- *Technology and commercial readiness level [TCRL]:*

TCRL gives a quantitative overview of the state of the technologies present in an energy system. Is a scale of how much the installation of a technology is feasible considering the well proven operation of existing power plants and, considering the commercial perspective, how is easy to get financial support for the technology by banks. These two indices are not invented but developed by ARENA [40] and Straub, J. [41]. Subsequently, they have been mixed together in a scale going from 0-14 in a second work [42] as it can be appreciated by Figure 18. TRL 9 and CRI 3 are considered at the same level. Totally, there are fourteen levels.

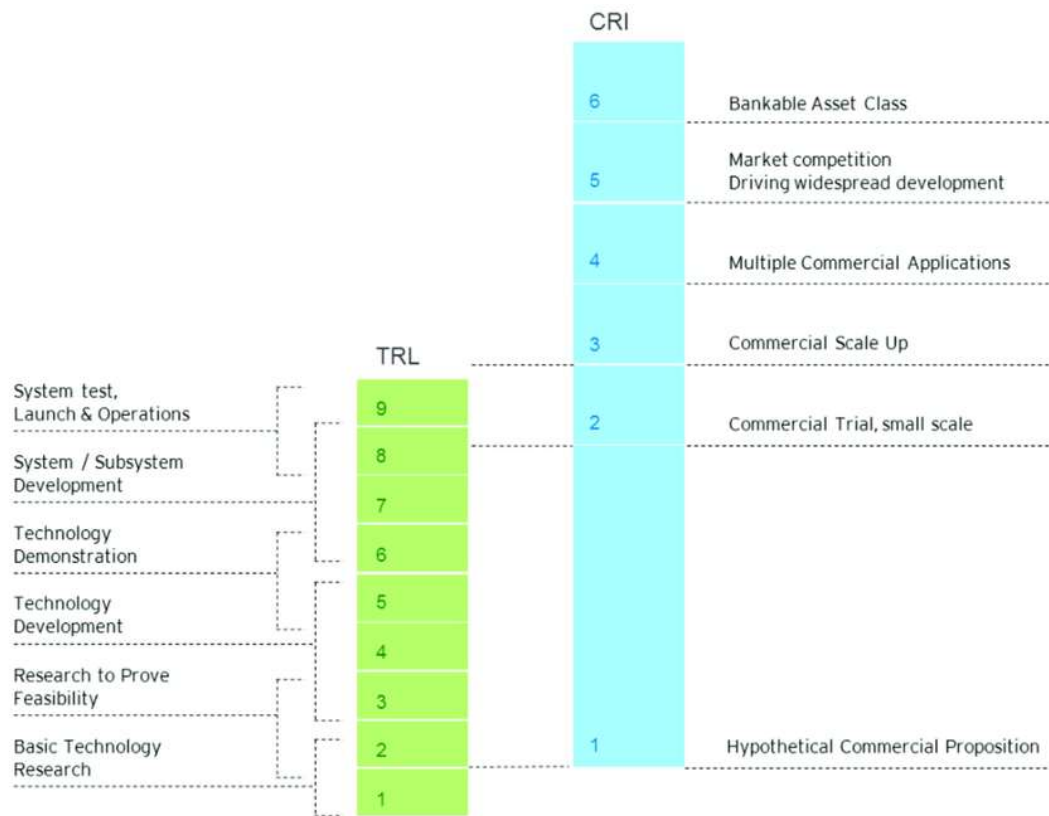


Figure 18. Technology and commercial readiness levels. [42].

- Reliability [Capacity Factor]:

The reliability of a technology is expressed by its capacity factor (CF). Indeed, CF is the annual generation of a power plant divided by the product of the capacity and the number of hours over a given period. In other words, it measures a power plant actual generation compared to the maximum amount it could generate in a given period without any interruption. A technology with a high CF value is very reliable, usually this value is close to one for dispatchable power plants.

- Diversification [Number of importer country for a power plant fuel]:

This parameter expresses the number of suppliers of a certain fuel needed in order to run a specific power plant. All the power plants with the same input fuel presents the same value for this parameter. Is a good indicator of how a certain plant is dependent by a single nation or more than one. In Table 7 is possible to see these considerations applied to the TIMES-Italy power sector.

Table 7. Security parameters for TIMES-Italy power sector.

Technology Description	TCRL [$\%$]	Reliability [CF]	Abundance [Years of proven resource]	Diversification [Nr. Of importer]
CYCLE with steam turbine USC (2006) >500 MW coal - AAT	14.00	80.00	114.00	10.00
Steam turbine USC-FGD (2006) < 2500 MW oil comb - AAT	14.00	80.00	47.00	5.00
Gas turbine < 80 MW with steam	14.00	75.00	51.00	7.00
Gas turbine < 300 MW	14.00	75.00	51.00	7.00
Combined cycle (gas turbine-2006) < 3000 MW - AAT	14.00	75.00	51.00	7.00
Biogas Agro-Zoo - BT	14.00	75.00	228.00	20.00
Biogas Waste - MT	14.00	75.00	228.00	20.00
Bioliquids plant	14.00	75.00	228.00	20.00
Biomass plant 5 cEuro - AT	14.00	75.00	228.00	20.00
Biomass plant 12 cEuro - AT	14.00	75.00	228.00	20.00
Biomass plant 5 cEuro - AAT	14.00	75.00	228.00	20.00
Biomass plant 12 cEuro - AAT	14.00	75.00	228.00	20.00
Solar with storage	13.00	26.00	228.00	20.00
PV roof plant	13.00	22.00	228.00	20.00
PV ground plant	13.00	18.00	228.00	20.00
Wind farm type A	11.00	25.00	228.00	20.00
Wind farm type B	11.00	25.00	228.00	20.00
Wind farm type C	11.00	25.00	228.00	20.00
Wind farm type D	11.00	25.00	228.00	20.00
Off-shore wind farm	9.00	27.00	228.00	20.00
Off-shore deep water wind farm	9.00	27.00	228.00	20.00
Mini hydro	14.00	50.00	228.00	20.00
Mini hydro >1 MW	14.00	50.00	228.00	20.00
Geothermal plant - AT	14.00	90.00	228.00	20.00
Geothermal plant - geocycles	14.00	90.00	228.00	20.00

Equity (or Social) parameters

This layer of the energy problem, as previously discussed, is the main debated since the direct accounting of social effects brings some difficulties due to the high number of steps when passing from a technical data to a social one. Indeed, parameters considered too far from the problem, like the impact of the energy system on occupation, are omitted. The only two parameters considered are the effects more related to human health described below.

- Health Impact potential [DALY/MWh]

This parameter is obtained for each technology from the Impact 2002+ framework for sustainability assessment [43]. Starting from midpoint LCA indicators as the ones used for the environmental layer, they are combined in a way able to account the damage caused by this indicators to the human health. Each midpoint indicator category is characterized by a midpoint reference substance for which emission are known thanks the NEEDS database. [44].

No. of LCI results covered [source]	Midpoint category	Midpoint reference substance	Damage category	Damage unit
769 [a]	Human toxicity (carcinogens + non-carcinogens)	kg _{eq} chloroethylene into air	Human health	DALY
12 [b]	Respiratory (inorganics)	kg _{eq} PM2.5 into air	Human health	
25 [b]	Ionizing radiations	Bq _{eq} carbon-14 into air	Human health	
22 [b]	Ozone layer depletion	kg _{eq} CFC-11 into air	Human health	
130 [b]	Photochemical oxidation [= Respiratory (organics) for human health]	Kg _{eq} ethylene into air	Human health	
			Ecosystem quality	–
393 [a]	Aquatic ecotoxicity	kg _{eq} triethylene glycol into water	Ecosystem quality	PDF * m ² * yr
393 [a]	Terrestrial ecotoxicity	kg _{eq} triethylene glycol into water	Ecosystem quality	
5 [b]	Terrestrial acidification/nutrication	kg _{eq} SO ₂ into air	Ecosystem quality	
10 [c]	Aquatic acidification	kg _{eq} SO ₂ into air	Ecosystem quality	Under development
10 [c]	Aquatic eutrophication	kg _{eq} PO ₄ ³⁻ into water	Ecosystem quality	Under development
15 [b]	Land occupation	m ² _{eq} organic arable land-year	Ecosystem quality	PDF * m ² * yr
38 [b]	Global warming	kg _{eq} CO ₂ into air	Climate change (life support system)	(kg _{eq} CO ₂ into air)
9 [d]	Non-renewable energy	MJ Total primary non-renewable or kg _{eq} crude oil (860 kg/m ³)	Resources	MJ
20 [b]	Mineral extraction	MJ additional energy or kg _{eq} iron (in ore)	Resources	

Figure 19. Overview of the Impact 2002+ Human Health calculation method. [43]

Referring to Figure 19, midpoint reference substances for plant activity are then translated in a damage unit, still defined for each unit of electricity produced by the plant. These last is used as final parameter. For a further discussion of the mathematics behind the DALY score calculation, the paper reading is suggested.

- Mortality [deaths/MWh]

Fatalities caused by power plants over a TWh of produced electricity is selected as a second parameter for the social layer. Energy accident related fatalities and estimated deaths caused by pollution are summed in order to define, on average, what are the risks of death associated to each unit of produced electricity. [45].

Data of these two parameters are directly resumed in Table 8.

Table 8. Equity (or Social) related parameters for TIMES-Italy power sector.

Technology Description	Human Health [DALY/MWh]	Mortality [Fatalities/MWh]
Biogas Agro-Zoo - BT	1.98	24.00
Biogas Waste - MT	1.98	24.00
Bioliquids plant	1.98	24.00
Biomass plant 12 cEuro - AAT	1.98	24.00
Biomass plant 12 cEuro - AT	2.72	24.00
Biomass plant 5 cEuro - AAT	2.72	24.00
Biomass plant 5 cEuro - AT	2.72	24.00
Combined cycle (gas turbine-2006) < 3000 MW - AAT	0.46	4.00
CYCLE with steam turbine USC (2006) >500 MW coal - AAT	1.92	100.00
Gas turbine < 300 MW	0.46	4.00
Gas turbine < 80 MW with steam	1.08	4.00
Geothermal plant - AT	0.00	0.00
Geothermal plant - geocycles	0.00	0.00
Mini hydro	0.00	1.40
Mini hydro >1 MW	0.00	1.40
Off-shore deep water wind farm	0.04	0.15
Off-shore wind farm	0.04	0.15
PV ground plant	1.86	0.44
PV roof plant	1.91	0.44
Solar with storage	0.20	0.44
Steam turbine USC-FGD (2006) < 2500 MW oil comb - AAT	1.01	100.00
Wind farm type A	0.04	0.15
Wind farm type B	0.04	0.15
Wind farm type C	0.04	0.15
Wind farm type D	0.04	0.15
PEM fuel cell system running on hydrogen 100 kW based	0.00	0.00

After having defined this wide list of indicators, is necessary to clearly explain how those sets of values will be used in order to build the final sustainability composite index of the energy scenario. Just a recap about all the data defined in this section, which are used in the next one:

- Power sector data (in particular, those of interest are the capacity factor, efficiency and lifetime of the TIMES-Italy technologies)
- Scenario data, in which we are interested only to the activity of each power production technology.
- Sustainability indices, related to the various aspects of the problem. In this case: Environment, Security and Equity.
- Sustainability parameters, defined for each TIMES-Italy power sector technology and related to the sustainability index category at which they belong.

2.4 Framework development

From here, the methodology for the ex-post sustainability assessment is explained. Objective of the developed framework is to evaluate, - starting from a database of LCA, non-LCA parameters and the scenarios data in terms of activity [MWh] of produced electricity - , the sustainability performances of the considered scenarios. The tools used for this analysis are the TIMES output data elaborator, Veda Back-End, and Matlab. Before proceeding, is necessary to adopt some conventions:

- In the mathematical notation, capitalization is used to denote a container, like a set or indexed parameter. Sets use only a single letter, so the lower case is used to represent an item from the set. For example, T represents the set of all technologies t and represents a single item from T .
- There are parameters that can be defined for other sets, for example the Water Use parameter will be finally defined for each technology and year. In order to denote that a value is referred to a specific technology and year, this last two elements will constitute the subscript of the main element. In this case:

$WU_{t,y}$ stands for Water Use of the technology t at year y

2.4.1 Data classification

Given that all the input data has been defined in the previous sections, here it follows a general classification of them, this is done in order to have a convention for the sets of data that will remain the same for all the analysis. First of all, in the previous sections the power sector has been defined. It is composed of technologies and data related to these lasts. Since in the Matlab tool technologies cannot be saved with their name, a single technology will occupy a position in a vector defined by a number going from one to the total number of technologies. In general, this is valid for all the sets of data.

t stands for technology, $t \in T[1, \dots N_t]$ with $N_t = \text{number of technologies considered}$

And we define years as:

y stands for year, $y \in Y[1, \dots N_y]$ with $N_y = \text{number of years}$

For the considered technologies we are interested in the capacity factor, lifetime and efficiency parameters which are indicated as:

$\eta_{t,y}$ stands for efficiency of $t \in T[1, \dots N_t]$ and $y \in Y[1, \dots N_y]$

$CF_{t,y}$ stands for capacity factor of $t \in T[1, \dots N_t]$ and $y \in Y[1, \dots N_y]$

$LT_{t,y}$ stands for lifetime of $t \in T[1, \dots N_t]$ and $y \in Y[1, \dots N_y]$

These three elements, defined for two indices, creates three 2D matrixes as:

$$\eta = \begin{bmatrix} \eta_{i,j} & \dots & . \\ \vdots & \ddots & \vdots \\ . & \dots & . \end{bmatrix}; CF = \begin{bmatrix} CF_{i,j} & \dots & . \\ \vdots & \ddots & \vdots \\ . & \dots & . \end{bmatrix}; LT = \begin{bmatrix} LT_{i,j} & \dots & . \\ \vdots & \ddots & \vdots \\ . & \dots & . \end{bmatrix} \quad (1)$$

where $i \in T[1, \dots N_t]$ and $j \in Y[1, \dots N_y]$

Then, scenarios data has been defined. Scenarios are characterized by several sets of data, like activity, capacity, costs and many others, but we are interested only in the activity. Activity, in this case the electricity produced by a power plant, is defined for each technology, milestone year of the scenario and also, for each scenario since the framework can evaluate a set of scenarios.

Scenarios are defined as:

s stands for scenario, $s \in S[1, \dots N_s]$ with $N_s = \text{number of scenarios}$

Now, activity can be defined as a three-dimensional matrix:

$$activity = \begin{pmatrix} a_{i,j,k} & \cdots & \cdot \\ \vdots & \ddots & \vdots \\ \cdot & \cdots & \cdot \end{pmatrix} \quad (2)$$

where $i \in T[1, \dots N_t]$, $j \in Y[1, \dots N_y]$ and $k \in S[1, \dots N_s]$

On the other side, there are data coming from the sustainability inventory. But, before defining them, is necessary to define the sustainability composite index, its related indicators and parameters in a very general way. Sustainability is a dimensionless real value (or better, a score) indicated by the acronym *SI* constrained between a maximum value *MS* and a minimum value *ms*, as below:

$$\{ SI \in \mathbb{R} \text{ t.c } ms \leq SI \leq MS \} \quad (3)$$

But, as previously explained sustainability value (or score, from now these two terms are interchangeable) is composed by several indicators:

ind stands for indicator, $ind \in IND[1, \dots N_{ind}]$ with N_{ind} = number of indicators

Expressed in the same metric:

$$\{ \forall ind \in IND[1, \dots N_{ind}], ind \in \mathbb{R} \text{ t.c } ms \leq ind \leq MS \} \quad (4)$$

Since we have several elements that constitutes the final sustainability score and all these elements are in the same metrics, the process that allow to account for all these elements in the sustainability score is the simple average:

$$SI = \frac{\sum_{i=1}^{N_{ind}} ind_i}{N_{ind}} \quad (5)$$

But, with a simple average all the indicators will have the same importance. Objective is to differentiate the importance of the indices thanks to a weighted average process. Then, sustainability can be calculated as in Equation 4.

$$SI = \sum_{i=1}^{N_{ind}} ind_i * w_i \quad (6)$$

$$\text{where } \sum_{i=1}^{N_{ind}} w_i = 1 \quad (7)$$

Now it comes the challenging part of the framework that is, to combine all the above-mentioned data in order to find for each scenario a unique value for the sustainability index. In order to move on is important to make a conceptual step. Indeed, is necessary to pass from parameters defined for each technology:

p_t stands for parameter $p \in P[1, \dots, N_p]$ defined for $t \in T[1, \dots, N_t]$

To impacts, related to parameters, defined for each year and scenario. To switch from one concept to the other is necessary to make an intermediate step. Indeed, sustainability parameters are data that applied to technologies activity creates impacts one impact for each type of parameter:

$$LCA \text{ Parameters } \left(\frac{\text{Parameter Value}}{MWh_{\text{electricity produced}}} \right) = \begin{pmatrix} p_{ij} & \dots & \cdot \\ \vdots & \ddots & \vdots \\ \cdot & \dots & \cdot \end{pmatrix} \quad (8)$$

where $i \in T[1, \dots, N_t]$, $j \in P[1, \dots, N_{LCA-P}]$

Or:

$$Non - LCA \text{ Parameters (Parameter value)} = \begin{pmatrix} p_{ij} & \dots & \cdot \\ \vdots & \ddots & \vdots \\ \cdot & \dots & \cdot \end{pmatrix} \quad (9)$$

where $i \in T[1, \dots, N_t]$, $j \in P[1, \dots, N_{N-LCA-P}]$

Where:

$$N_{LCA-P} + N_{N-LCA-P} = N_p \quad (10)$$

Parameters data must be elaborated with activity of the plants in order to calculate the impacts of the power sector. Conceptually, each scenario will have a set of matrices, one for each parameter (and then, for each impact) that describe the value of the impact caused by each technology in each simulated year. It is built like this:

$$Impact_m = \begin{pmatrix} iv_{i,j} & \cdots & . \\ \vdots & \ddots & \vdots \\ . & \cdots & . \end{pmatrix} \quad (11)$$

where $i \in T[1, \dots N_t]$, $j \in Y[1, \dots N_y]$ and $m \in P[1, \dots N_p]$

The general element of the impact matrix is obtained as:

$$iv_{m,i,j} = a_{i,j} * p_{m,i,j} \quad (12)$$

where $i \in T[1, \dots N_t]$, $j \in Y[1, \dots N_y]$ and $m \in P[1, \dots N_p]$

So, we need parameters defined not only for the technologies, but also for the future years. In order to build this set of data is necessary to harmonize data between TIMES and LCA-parameters. This refers to taking TIMES data for efficiency, capacity factor and lifetime and modifying the LCA data, which allows considering the improvement in time and add the dynamic component to LCA-data. For non-LCA data parameters are assumed constant through the years.

2.4.2 Harmonization

The desired situation is to get one matrix for each impact, with impacts defined for each technology and for the milestone years, including the base one.

2 Kind of parameters:

- LCA parameters are assumed varying with the technological improvement

$$LCA\ Data \propto f(\eta, CF, Lifetime)$$

Harmonization is performed by taking the average growth rate of the before mentioned parameters, reducing by the same percentage the LCA impacts:

$$Average\ GR_{t,y} = \frac{1}{3} \left(\frac{\eta_{t,y} - \eta_{t,1}}{\eta_{t,1}} + \frac{CF_{t,y} - CF_{t,1}}{CF_{t,1}} + \frac{LT_{t,y} - LT_{t,1}}{LT_{t,1}} \right) \quad (13)$$

$$LCA\ Impact_{t,y} = LCA\ Impact_{t,1} * (1 - Average\ GR_{t,y}) \quad (14)$$

The rationale behind this process is related to the way unitary life cycle impacts are calculated for electricity power plants. In fact, in order to calculate these last the life cycle impact of a reference plant is divided by its overall life cycle electricity production:

$$\begin{aligned}
\text{Unitary impact} \left[\frac{\text{impact}}{\text{MWh}} \right] &= \\
&= \frac{\text{Life cycle impact (construction, operation, and of life, supply)}}{\text{Life cycle electricity production}}
\end{aligned} \tag{15}$$

Since the life cycle electricity production increase when increasing the capacity factor and the lifetime there is a reduction of the unitary LCA impact. Also, a higher efficiency, especially for a fuel combustion power plant, causes a lower require of supply. Given that the LCA unitary impact is only related to the output of the plant, in order to account for the minor impact caused by a decreasing need of supply also the efficiency has been included in the harmonization process.

For renewable energy sources where no input is needed the same equation has been used, even if accounting for the efficiency zero grow rate decrease the weight of the other two components, and this cause a little error. This error is accepted since dividing the formulation for each type of technology will require a too case-specific formulation of the code, which instead aim at being as flexible as possible.

- Non LCA parameters, these are assumed constant through the years

$$\text{non} - \text{LCA Impact}_{t,y} = \text{non} - \text{LCA Impact}_{t,1} \tag{16}$$

This process allows the creation of a matrix for each impact category, with impact values defined for each technology and year.

$$\begin{aligned}
\text{Parameter}_m &= \begin{pmatrix} p_{i,j} & \cdots & \cdot \\ \vdots & \ddots & \vdots \\ \cdot & \cdots & \cdot \end{pmatrix} \\
\text{where } i &\in T[1, \dots N_t], j \in Y[1, \dots N_y] \text{ and } m \in P[1, \dots N_p]
\end{aligned} \tag{17}$$

2.4.3 Impact assessment

Objective is now to obtain a general matrix in which the values are the impacts, divided by category and years for each scenario. Impacts are obtained by multiplying each technology activity for its unitary impacts.

Before entering in the detail of this part is necessary to make an important consideration. Multiplying technology parameters for the activity means obtaining higher impacts for those scenarios which

presents a high degree of electrification, because the overall activity for the electricity production plants will be higher. From a simple post-processing point of view this is not a problem but also, is interesting to see what the differences among scenario impacts are when changing the overall electricity production. The problem is that impacts not caused by the power sector are totally unaccounted, like the ones caused by the heat production or other commodities. Given that aim of this work is to implement the sustainability metric inside the TEMOA energy model, an overall electricity production impacts accounting can result in a de-electrification of the energy scenarios simulated. Indeed, other commodities will be used to satisfy the demand because they will cause a lower electricity production and subsequently, lower impacts. (e.g. in the transport sector). In order to solve this problem is necessary to have the sustainability score related to the power production technologies mix, but not to the overall electricity production. In this way is possible to have a comparison on how sustainable electricity production is, without referring to the total amount produced. Is possible to achieve this target by considering the activity share instead of the overall activity:

$$ActivityShare = \begin{pmatrix} aS_{i,j,k} & \cdots & \cdot \\ \vdots & \ddots & \vdots \\ \cdot & \cdots & \cdot \end{pmatrix} \quad (18)$$

$$where i \in T[1, \dots N_t], j \in Y[1, \dots N_y] and k \in S[1, \dots N_s]$$

By doing this step, is possible to obtain for each parameter, an average unitary impact for the year of each scenario. Again, take as an example the Water Use:

$$WU_{i,j,k} = \sum_{i=1}^{N_t} WU_{i,j,k} * aS_{i,j,k} = \left[\frac{Water Use}{MWh} \right] \quad (19)$$

In this way is possible to obtain a global average parameter defined for each year of each scenario. From here, let us consider we are evaluating a single scenario, so, let us neglect the k term for the moment.

The abovementioned procedure can be easily repeated for all the years and for all the parameters considered in this analysis, creating a matrix in which the global average parameters are calculated for each year. In order to perform this step we simply need the *ActivityShare* matrix multiplied for the Np impact parameters matrixes:

$$Parameter_m = \begin{pmatrix} p_{i,j} & \cdots & . \\ \vdots & \ddots & \vdots \\ . & \cdots & . \end{pmatrix} \quad (20)$$

where $i \in T[1, \dots N_t]$, $j \in Y[1, \dots N_y]$ and $m \in P[1, \dots N_p]$

This process creates a N_p number of matrixes, each of them related to an impact p :

$$Impact_m = \begin{pmatrix} imp_{i,j} & \cdots & . \\ \vdots & \ddots & \vdots \\ . & \cdots & . \end{pmatrix} \quad (21)$$

where $i \in T[1, \dots N_t]$, $j \in Y[1, \dots N_y]$ and $m \in P[1, \dots N_p]$

Now, for each matrix is necessary to condense data into a single string, by eliminating the division of the impact by technology. Indeed, we are interested in the overall impact value, not in the single technology impacts. Then, data are summed in a new vector like:

$$TotalImpact_m = \sum_{i=1}^{N_t} imp_{i,j} = (imp_{BASEYEAR} \dots imp_{LASTYEAR}) \quad (22)$$

where $i \in T[1, \dots N_t]$, $j \in Y[1, \dots N_y]$ and $m \in P[1, \dots N_p]$

Finally, all the *TotalImpact* vectors are stored in a unique matrix:

$$IMP = \begin{pmatrix} imp_{i,j} & \cdots & . \\ \vdots & \ddots & \vdots \\ . & \cdots & . \end{pmatrix} \quad (23)$$

where $i \in P[1, \dots N_p]$ and $j \in Y[1, \dots N_y]$

In this final matrix, all the different impacts of all the energy dimensions are stored in a single matrix for each scenario. In each row there is a different impact, defined for each year in the columns.

For the moment, all the data stored in *IMP*, are vectors characterized by different metrics. In fact, in each row we have global average parameters for each year, where each parameter has its own metric. In necessary to pass to a single metric matrix.

2.4.4 Normalization

After collecting input data for the sustainability assessment in the *IMPACTS* matrix, we must do some pre-processing to ensure comparability of impact and thus, making it useful for evaluation process of sustainability score. Indeed, in order to find a sustainability score we have to define what are the sustainability score boundaries, then, transform the absolute quantities of the impact indicators into dimensionless amounts constrained in the sustainability score boundaries.

A useful method to re-shape data in a common scale is the normalization. In general, normalization is a transformation process to obtain comparable input data by using a common scale and this process is very famous in all the MCDA studies from which this work has some points in common. Since objective is to evaluate the technology mix accounting for those impact values, we are not interested in the absolute value of them but in their relative difference between the best and the worst possible cases. So, is possible to bring all the impacts on the same scale.

In this case, the normalization process takes a value “ z ” constrained into a space limited by X and Y values, transforming it into a value “ o ” constrained into a space limited by MS and ms values. X & Y are the boundaries of the impact considered and they represent the best and the worst impact for each impact class. MS & ms are instead, the boundaries of the sustainability score.

$$\begin{bmatrix} Y \\ z \\ X \end{bmatrix} \rightarrow \begin{bmatrix} MS \\ o \\ ms \end{bmatrix} \quad (24)$$

where the impact value $i \in [X, Y]$ and the *NormImpact* $\in [ms, MS]$, and

where MS and ms are the upper and the lower boundaries of the sustainability score

There are three important things to consider before proceeding with the normalization:

- The normalization method
- The selection of the upper and lower boundaries
- The type of parameters

Starting with the normalization method, two possible options have been tested before applying one of them at the final version of the framework: The min-max scaling and the zero scaling. A min-max scaling normalization is typically performed via the following equation:

$$x_{scaled} = \frac{x - x_{min}}{x_{max} - x_{min}} \quad (25)$$

In the zero scaling the formula is the same, but the minimum value of x is the zero.

Ideally, a zero-impact energy system would be the ideal case, so this may bring the analysis in the direction of a zero-scaling normalization but, since we are in a real world, for each impact class we must refer to the best available option. Then, we must refer the limits to technological existing limits. For this reason the min-max scaling has been used given that, dealing with technologies, there is no “ideal case” but a set of options.

Selection of boundaries is done using a criteria called “ALARA”, that means “as low as reasonably achievable” and its opposite concept “AHARA”, that means “as high as reasonably achievable”. Applied to the power sector, the minimum value of a certain impact class is reached when the technology that presents the lowest value for those class produces all the electricity (has a share equal to 1). The opposite happens when looking for the maximum value of an impact.

Notice that there are impacts that follows a logic called “The lower the better”, as it happen for all the LCA parameters. So, the lower is the impact value and the better is the sustainability situation. There is an opposite situation that happens specifically for the security parameters, in particular for TRL, CF, Abundance and Diversification, in which the logic is “The higher the better”. These two types of parameters require a different normalization formula. Remember that we want the Sustainability score to be “the higher the better” so, when the impact is a of type “the lower the better” we should apply a reversed normalization as in the formula below:

$$\frac{z - X}{X - Y} = \frac{o - MS}{MS - mS} \Rightarrow o = mz + q \quad (26)$$

Instead, when the parameter is already in a “the higher the better” scale, the formula is:

$$\frac{z - X}{X - Y} = \frac{o - mS}{mS - MS} \Rightarrow o = mz + q \quad (27)$$

where MS and ms are the upper and the lower boundaries of the sustainability score

Differences between the two methods are shown in Figure 20 where a generic impact vector going from 100 to 1000 has been normalized following the two approaches. In this case mS and MS are respectively equal to zero and one.

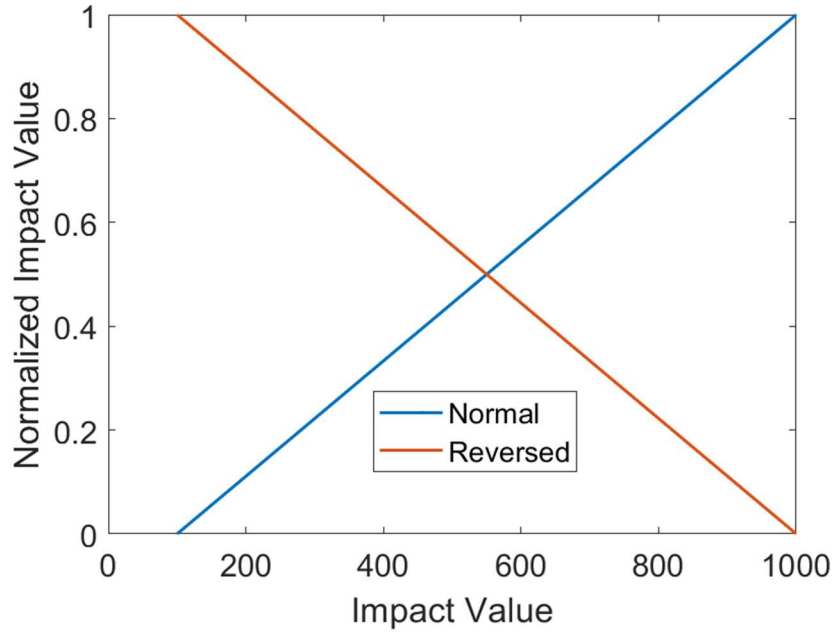


Figure 20. Normalization methods: comparison between normal and reversed min-max scaling.

By applying the normalization, both in the reversed and normal mode depending on the type of impact, we produced the final matrix:

$$NORMALIZED\ IMPACTS = \begin{pmatrix} niv_{i,j} & \cdots & . \\ \vdots & \ddots & \vdots \\ . & \cdots & . \end{pmatrix} \quad (28)$$

$$where\ j \in Y[1, \dots, N_y] \text{ and } i \in P[1, \dots, N_p]$$

With all the values constrained between 0 and 1 and already scaled in a “the higher the better” logic. The last step is to combine those values in order to calculate the indices that finally constitutes the sustainability score.

2.4.5 Weighting

Let us recall the sustainability formula:

$$SI = \sum_{i=1}^{N_{ind}} ind_i * w_i \quad (29)$$

$$\text{where } \sum_{i=1}^{N_{ind}} w_i = 1 \quad (30)$$

The sustainability value, as the values of its indicators, are unique scores calculated for each scenario. For this reason, these lasts must account for the behavior of the scenario through all the milestone years. The problem relies in the normalized impacts, that instead are defined for every single year. Is necessary to find an operator which acts as a “bridge” between the yearly defined normalized impact and the sustainability indicators characterized by a unique value. Thanks to the integral operator, each index component of the final sustainability score, can be calculated as:

$$ind_k = \int_{i=1}^{N_{years}} \sum_{j=1}^{N_{pi}} NormImpact_{i,j} * wp_{j,k} \quad (31)$$

$$\text{where } \sum_{j=1}^{N_{pi}} wp_{j,k} = 1 \quad (32)$$

where N_{pi} is the number of impacts assigned to the index i and $w_{j,k}$ is the weight assigned to the parameter j belonging to the index k

From these equations is easy to recognize that there are two different types of weights. The first order type is associated at the energy aspect considered (environment, social or security index). The second type of weights is related to the parameters inside one of the three energy indicators (environment, social or security index). The combination of parameters and second order weights creates the indicators, as the combination of first order weights and indicators creates the sustainability score. The weight attribution is not fixed, but the only condition is that the sum of all the weights (for the single type) is one.

Now, notice that indicators in Equation 28 are not defined over a year, while the different *NormImpact* instead they are. Indeed, indicators creates sustainability score which is a single value for each scenario. Is also possible to define a sustainability score of the year inside the scenario:

$$si_{years} = \sum_{i=1}^{N_{ind}} yind_{i,year} * w_i \quad (33)$$

And the final sustainability score will be:

$$SI = \frac{1}{(Y_N - Y_1)} \int_{y=1}^{N_{years}} si_y \quad (34)$$

Or:

$$SI = \sum_{i=1}^{N_{ind}} ind_i * w_i \quad (35)$$

Where ind_i is calculated as:

$$ind_i = \frac{1}{(Y_N - Y_1)} \int_{y=1}^{N_{years}} yind_i \quad (36)$$

In conclusion, by applying the integral mean value theorem is possible to switch from yearly defined indices and sustainability score to a final value for each scenario.

2.5 Results

In this section the outcomes of the sustainability assessment applied at the TIMES-Italy power sector are discussed. Purpose is to show not only the final graphs related to the sustainability score, but also to give a practical overview of the mathematical framework described above, in particular at what numerically happen when running the normalization and the harmonization processes.

Proceeding chronologically, harmonization is the first step performed by the framework. It takes as input technical data (efficiency, lifetime, capacity factor) for each technology and reduces the LCA parameters accounting for the technological improvement, as described in Equation 12. Applying this procedure mathematically means multiplying the LCA parameter of the technology for a reduction coefficient defined for each year. By following this procedure is possible to reduce the LCA impacts related parameters for some technologies by almost 20%, as it can be appreciated in Figure 21. Technology legend has been omitted due to the too high number of technologies considered. Purpose of the plot is just to show the percentage of reduction obtained.

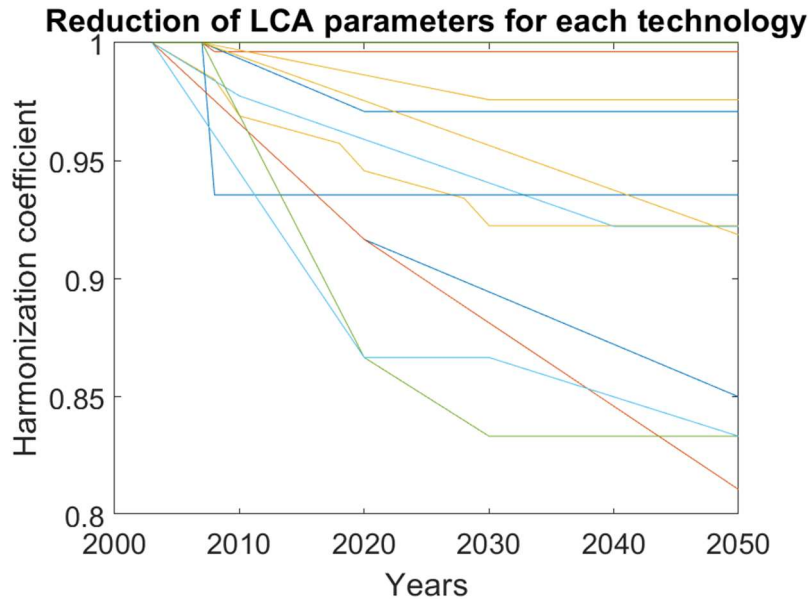


Figure 21. Harmonization Coefficient for TIMES-Italy power sector technologies.

Once applied the harmonization process the yearly-defined impact parameters are obtained for each technology. Now, is possible to proceed with the impact assessment. Assessing the impact of the current power sector means, for every year, combine the technology impact parameters with the activity share of them, creating an average impact parameter of the energy system. An example of this process, again taking water use a reference like in Equation 19, is the one here below:

$$WU_{y,s} = \sum_{i=1}^{N_t} WU_{i,y} * AS_{i,y,s} = \left[\frac{Water\ Use}{MWh} \right] \quad (37)$$

For each impact type and scenario it is possible to create a vector which stores all the average impact parameter of the energy system for each year. In Figure 22 is shown the Water Use impact for the three scenarios considered.

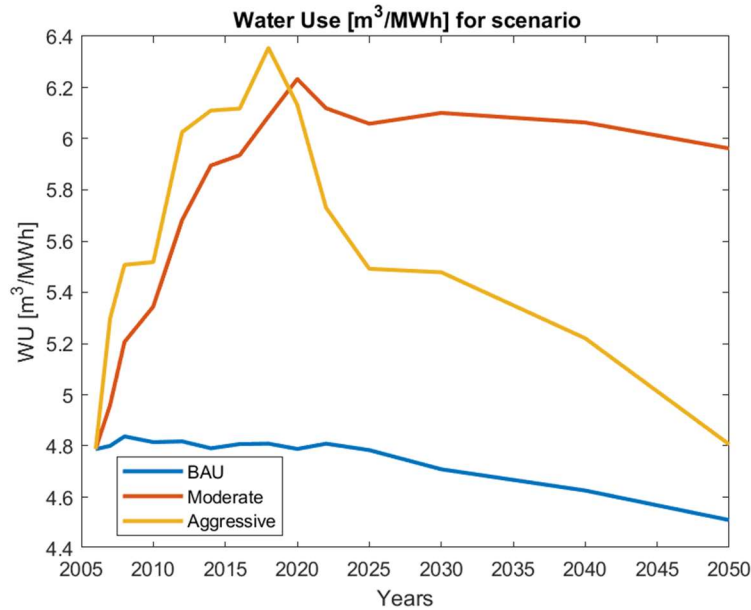


Figure 22. Water Use impact parameters for TIMES-Italy scenarios.

Figure 23 highlights the evolution of the scenarios Water Use global parameter, which indicated the average water consumption related to the production of 1 MWh of electricity during the years for the scenarios considered.

In this case the low carbon scenarios presents a worst behavior with respect to the business as usual, but it has to be noticed that the scale starts from 4.4 [m³/MWh] and the maximum relative difference is around 30%. The problem when dealing with absolute values is that we cannot establish how good or bad the situation is with respect to the ideal one. In order to evaluate each impact, and finally the sustainability score the next step is the normalization process. Recalling Equation 22 objective is to shift the Water Use limit values. In particular, we want to shift the worst and the best possible average impact parameter of the energy system. Since we want to minimize the impact, the best solution will be the case in which the technology with the lowest water consumption has a share equal to one. Worst and best solution will respectively occupy the value 0 and 1. Indeed, this impact parameter is of “The lower the better” type, thus, one should indicate the best situation because in the end 100 will be the maximum value of sustainability. (And vice versa for 0). So, we should apply the reversed normalization of Equation 24. Is important to notice that the normalization process limits (the best

and the worst value) comes from the power sector, so the evaluation is independent by the scenarios considered. In Figure 23 normalized Water Use is shown:

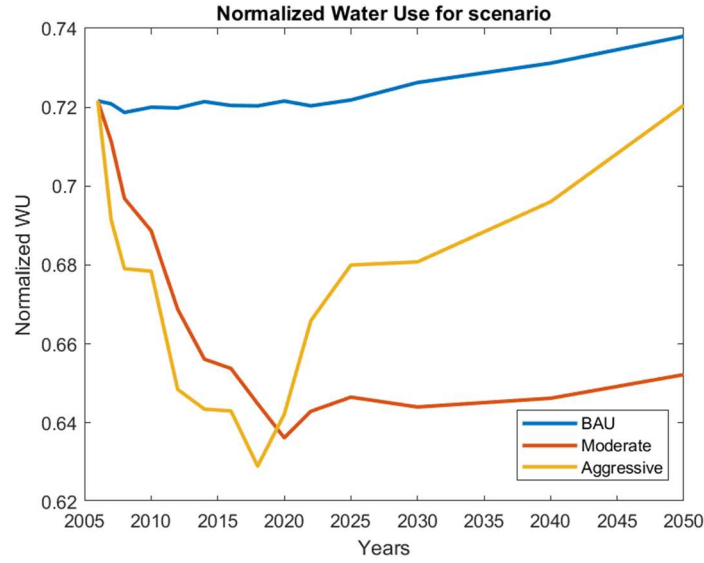


Figure 23. Normalized Water Use impact parameters for TIMES-Italy scenarios.

Is visible how all the Water Use normalized values are in a good level of the scale, even if low carbon scenarios present lower impact values and then, higher normalized values. Also, is interesting to highlight the change of trend that the Moderate and Aggressive scenarios have after 2020, years in which a technological change begin referring to Figure 16 and Figure 17.

Once analyzed the methodological steps, before moving to the results is necessary a fast recap on the evaluation system. Let us recall Equation 4 and Equation 28, by substituting the ind_i term of the latter in the former:

$$SI = \sum_{i=1}^{N_{ind}} \left(\int_{y=1}^{N_{years}} \sum_{j=1}^{N_{pi}} NormImpact_{j,y} * wp_{i,j} \right) * w_i \quad (38)$$

This is the final formulation of the sustainability score in which all the sets of data are condensed. Is possible to highlight the presence of two weight types. In particular, the one outside the brackets is the first order weight associated to the sustainability indices, while the second one (inside the brackets) is related to the normalized impacts. In the sustainability problem weights are decision variables and the choice must be made considering several aspects. In this first case, first and second order weights are assumed as in Table 9. At the end of this section, a discussion of the weights influence on the final outcomes is present.

Table 9. Weights assigned to indicators and parameters.

Environment	0.50	Security	0.30	Equity	0.20
GWP	0.16	TRL	0.25	Human Health	0.50
AP	0.16	Reliability	0.25	Mortality	0.50
EP	0.16	Abundance	0.25		
Land Use	0.16	Diversification	0.25		
Water Use	0.16				
Noise					
Pollution	0.10				
Waste					
Creation	0.10				

Once defined the weight, all the ingredients necessary at the framework to calculate the sustainability score are present. In Figure 24 the paths of the sustainability score through the years for each TIMES-Italy scenario are plotted:

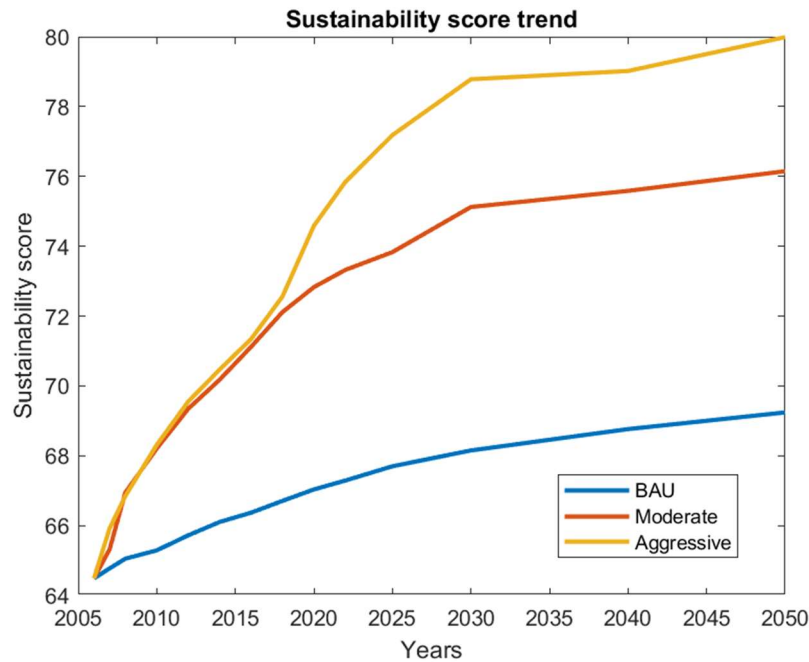


Figure 24. Yearly sustainability score for TIMES-Italy scenarios.

Simulation starts at year 2006 and at the beginning, the situation is the same for all the three scenarios. Then, for what concern the Business as Usual, since the aim of this scenario is to keep the electricity mix constant, the sustainability score slightly moves up due to the little technological improvement it experiences in the harmonization process. Variations are also justified by Figure 15 in which the energy mix is not perfectly constant as well. Increase of sustainability is always a combination of

technological change and technological improvement (harmonization). Looking at Moderate and Aggressive the storyline is different, till 2020 they have a similar path, but from 2020 Aggressive starts experiencing a higher reduction of oil and gas (referring to Figure 17) causing an increase of the sustainability.

Is important to notice that, even if the maximum level is one hundred, this value is never reached. Indeed, this value an ideal limit infeasible from a technological point of view. Having a scenario with a sustainability score equal to 100 will imply that all the indexes and normalized impacts are all equal to 1 (100 is just an extension of the 0-1 scale to improve the visualization). This situation implies that each impact is caused by the whole electricity production supplied by the less impacting technology, but since different technologies are the best for different impacts, the above-mentioned situation is unfeasible.

Nevertheless, this sustainability metric is a good tool to evaluate scenario's performance, especially when compared to other situations. The fact that this metric is independent from other scenarios but only to the power sector constitutes a general framework for scenario evaluation, which is also very useful for the next part of endogenous integration. In particular, the tool can be used to provide such intuitive and clear information about the actual and future status of an energy situation when compared to other possible solutions. Ideally, Figure 25 visualization can be integrated as interface in a model generator in order to have a fast check on the sustainability situation of the different alternatives.

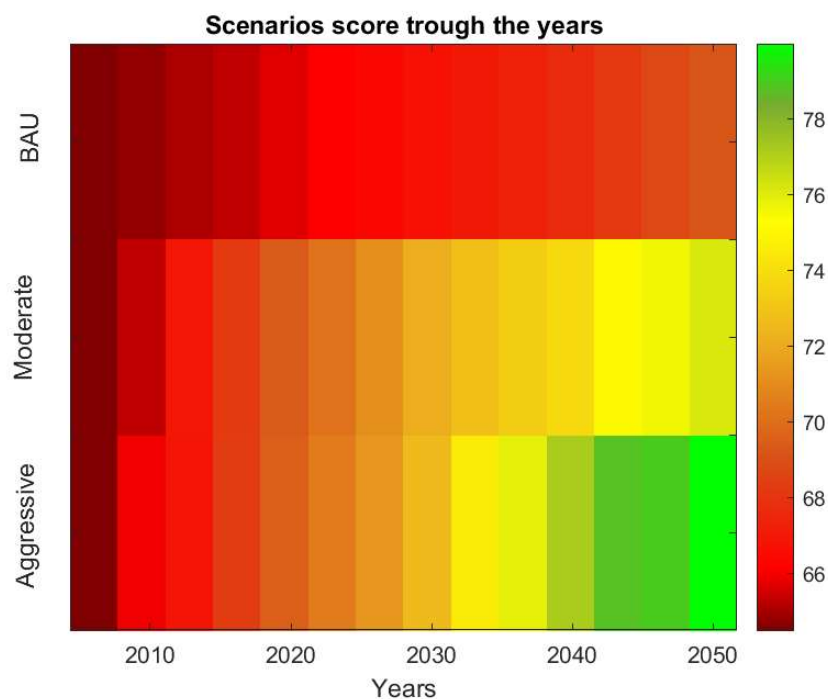


Figure 25. Redlight/Greenlight evolution of the sustainability score for TIMES-Italy scenarios.

Recalling Equation 31 and Equation 32, the overall sustainability score is the integral average of the yearly one:

$$SI = \frac{1}{(Y_N - Y_1)} \int_{y=1}^{N_{years}} si_y \quad (39)$$

SI can also be written as the weighted sum of the indices:

$$SI = \sum_{i=1}^{N_{ind}} ind_i * w_i \quad (40)$$

Equation 32 and 31 can be summarized in the Figure 26 visualization. The picture shows the final score of the three TIMES-Italy scenarios, again extended to a 0-100 scale instead of 0-1. As expected by looking at Figure 24 the Aggressive scenario is the one characterized by the highest score, given that the area below its curve in the yearly score is the highest.

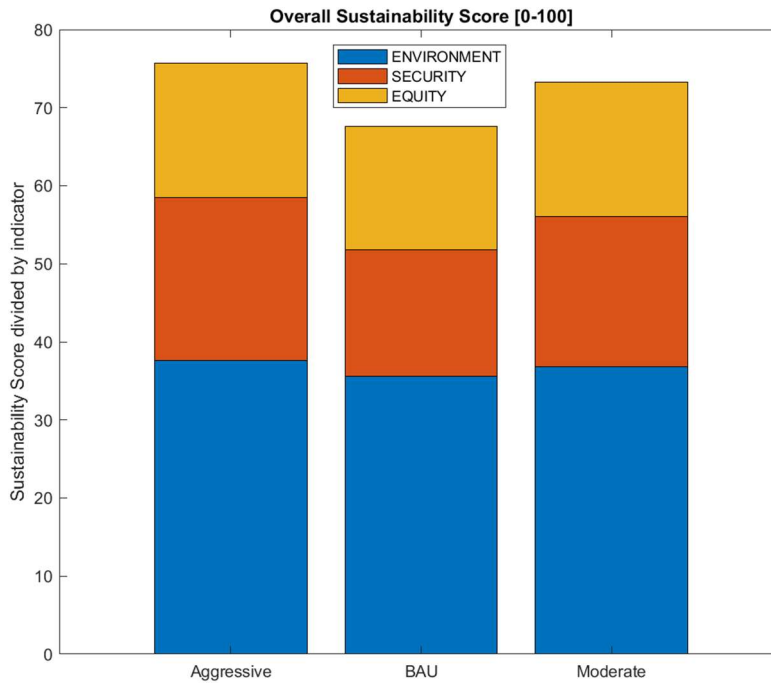


Figure 26. Overall Sustainability Score for TIMES-Italy scenarios.

This visualization is fundamental for the next part because it highlights an important aspect: Sustainability metric confirms benefit of low carbon scenarios, and this consideration is important for two reasons. First of all, it tells us that we can integrate emission reduction targets with beneficial

environmental and security effects. Second, if a higher sustainability score is assigned to scenarios with a high degree of decarbonization, once the score is integrated inside the model, optimizing with respect to the sustainability will mean driving the energy system towards low carbon solutions.

Another important consideration that perfectly fits with Figure 26 is related to the difference, in terms of numerical value, existing between the three scenarios overall sustainability scores. Is clearly visible that the gap between the best and the worst scenario is not really enhanced by this metric. These may constitute a problem when integrating the framework inside a model since a low difference in the score means a low variation of the objective function of the model between two scenarios. A thin gap may be neglected by the model and this situation is to avoid. Is then necessary to study in detail when the difference between the scenarios is abated. Starting from the raw impact data, a scenario impact assessment follows a normalization process, a first calculation of the yearly sustainability score and finally an integration in order to find the overall score.

The methodology applied in order to analyze the difference abatement in the process steps rely on the relative difference concept:

$$\delta_y = abs \left\{ \frac{Impact_{aggressive} - Impact_{BAU}}{\min(Impact_{aggressive} - Impact_{BAU})} \right\} \quad (41)$$

Relative difference has been calculated starting from the impacts as in Equation 38, obtaining one value for each impact and then making the average:

$$\delta_{avg,y} = \frac{\sum_{i=1}^{N_p} \delta_i}{N_p} \quad (42)$$

Since the steps that bring to the final sustainability score are the following:

Impacts → Normalized Impacts → yearly score → Overall score

The same Equation 38 and Equation 39 have been applied to all the other steps, obtaining for the defined framework the yearly trend of the relative differences along all the steps of the process, they are reported in Figure 27.

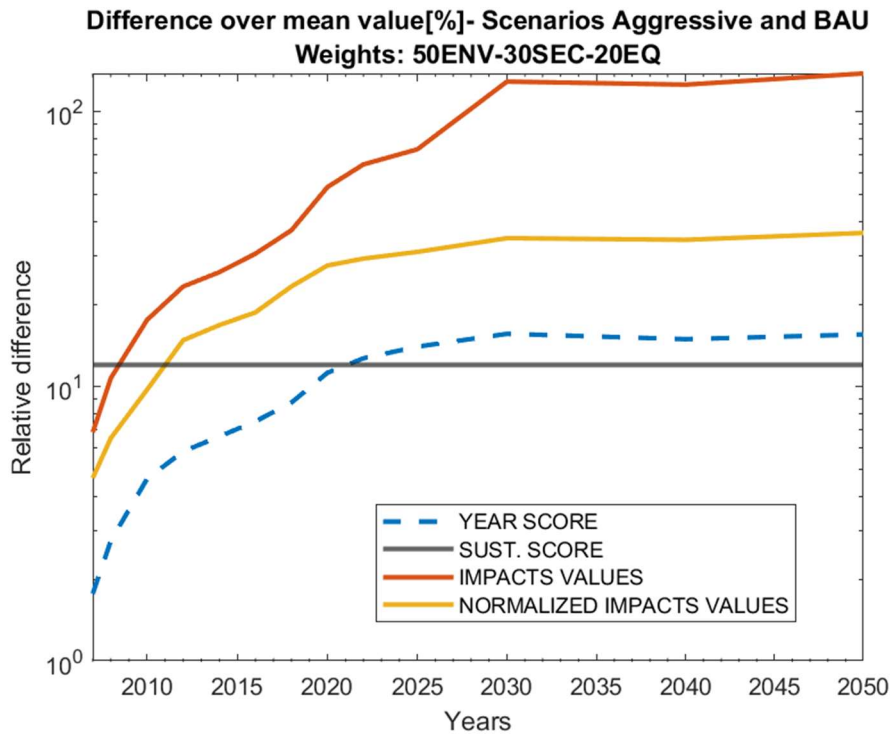


Figure 27. Relative difference trends along the several steps of the process.

As it can be noticed, impacts have orders of magnitude of difference in origin, but this gap is progressively abated by the several processes of the framework. Nevertheless, differences between scenarios are still in the order of 10% and this is a difference which is relevant for the model. Also, we will see how is possible to make this variation to be considered in a relevant way thanks to a proper formulation of the model objective function. In conclusion, the gap abatement is in general a problem when building metrics that relies on normalization and weighting methods, but in this case a 10% variation is an acceptable result, also considering that the energy scenarios analyzed are not drastically different.

These last considerations open at the second part of this work, which aims at integrating this metric inside TEMOA.

Chapter 3: A new optimization paradigm for sustainability assessment

Purpose of this part is to describe the steps that has brought to the endogenous integration of the sustainability indicator inside TEMOA, and subsequently to the direct accounting of this last inside the model objective function. Concerning the first part, integrating means performing the same procedure previously done ex-post directly inside the model. Then, for each generated scenario TEMOA must be able to calculate the sustainability index. This step has been implemented creating a separated structure which aim is to derive from all the impact sets a general impact score for each technology. Subsequently, the technology impact score is taken as input in the core part of the model and the final score is computed by multiplying this last for the activity of the electricity production technologies. This procedure, which may seem different in nature from the ex-post analysis, is the same but formulated in a different way which is easier to be implemented inside the model. Details of this part will be explained in the relative section.

All the described procedure is integrated inside a simplified version of the TEMOA-Italy which refers only to the power sector.

After having inserted the sustainability evaluation inside TEMOA and applied it to the TEMOA-Italy, the evaluated impact/sustainability final value should be integrated inside the objective function to perform a sustainability-economic oriented optimization. In this part a description of the multi-objective optimization techniques which are used is present. In particular, the weighted sum and the ϵ -method have a key role in this analysis and the reason will be clearly explained. The two optimization techniques are integrated in two different versions of the TEMOA-Italy. Finally, results of the selected approach will follow with a detailed discussion on the results and the issues related with the weighted sum approach.

3.1 The TEMOA-Impact module: Integration of the framework

This first part describes in detail the rationale and the procedure followed for the integration of the sustainability evaluation method inside TEMOA. Before start explaining anything is necessary to clarify a major difference between the ex-post analysis and the endogenous integration. When performing a post-processing analysis results are known a priori an impact related parameters are directly multiplied for the activity share known data. If the aim of this integration inside TEMOA is to drive the evolution of the energy scenarios, the integration of the impact related parameters should be done in such a way that these lasts are related to the decision variables of the model.

In order to better understand this part is necessary to highlight how the TEMOA model works. As a model, it is characterized by parameters and variables. Simplifying the terms, parameters are numerical values which represent an attribute (a cost, an emission factor, a discount rate) defined for several time steps (day/night, season/year) of a certain process, if not different specified parameters are in general fixed. Variables are instead mutable entities that represent the operation of the process in the system, like activity and capacity. The TEMOA model generates several equations in the form:

$$f(v_1, \dots v_n) = A * v_1 + \dots K * v_n \quad (43)$$

Where $A, \dots K$ are the parameters and v are the generic variables. The generated expressions go inside a solver, which modify the variable values in order to find a system configuration that minimize the objective function which is, in turn, an expression formed by variables and parameters. This explanation clarifies what should be the approach when dealing with sustainability inside the model. Indeed, sustainability must be written inside TEMOA as an expression composed by parameters and variables. This is a first critical point to keep in mind.

A second important consideration rely on the optimization approach that must be integrated. If the aim is to integrate a different objective, totally separated by the economic objective function, there are no important issue to discuss. A simple new objective equation implementation is required and then this last is solved separately from the economic objective function that characterize TEMOA [21]. But, in this case, aim is to integrate the sustainability inside the current economic objective function, the reason of this choice will be later explained. The simultaneous integration of two objectives in the same equation implies that both the targets must be minimized or maximized, but the process must happen for both of them. Is unfeasible to have a single objective function composed

of two terms, in which one should be maximized and the other minimized, because the optimization acts with respect to the total value. Unfortunately, the economic-sustainability optimization falls in the abovementioned case, since the economic cost of the system must be minimized while the sustainability maximized.

After this discussion, there are two evident problems in the actual formulation of the sustainability:

1. The sustainability indicator, in opposition with the economic cost, follows a “The higher the better” rule. Solution relies in the inversion of the index, creating a “unsustainability” indicator, which requires a minimization.
2. According to Equation 40, sustainability should be calculated thanks to an expression which contains variables and parameters. The actual sustainability calculation framework looks very similar to Equation 40 due to the presence of impact parameters that are multiplied for activity but. after that, impacts follow a normalization procedure, which implementation is unfeasible in the model. Indeed, model needs a direct expression and not a set of steps. A novel formulation should be defined.

To solve these two aspects, let us consider the sustainability formulation of Equation 35:

$$SI = \sum_{k=1}^{N_{ind}} \left(\int_{i=1}^{N_{years}} \sum_{j=1}^{N_{pi}} NormImpact_{i,j} * wp_j \right) * w_k \quad (44)$$

Where the term *NormImpact* could be decomposed, following the normalization formula, as:

$$NormImpact_j = \frac{\sum_{t=1}^{N_t} P_{t,j} * AS_t - \min(P_j * 1)}{\max(P_j * 1) - \min(P_j * 1)} \quad (45)$$

This because the normalization of a certain impact is performed with respect to the bottom and top limit values that would be obtained by producing all the electricity respectively with the best and the worst power production technologies for the considered impact. Indeed, producing all the electricity with a certain technology means having an activity share equal to one and that is what happen in the brackets of min () and max () of Equation 42.

By inserting Equation 42 in 35 we get:

$$SI = \sum_{i=1}^{N_{ind}} \left[\int_{y=1}^{N_{years}} \sum_{j=1}^{N_{pi}} \left(\frac{\sum_{i=1}^{N_t} P_{t,j} * AS_t - \min(P_j * 1)}{\max(P_j * 1) - \min(P_j * 1)} * wp_{i,j} \right)_{i,j} \right] * w_i \quad (46)$$

Now, is possible to observe that if we neglect the activity share from the analysis, by eliminating the term AS and the I in the red normalization part, and also by eliminating the summation related to the technologies N_t in blue (that is the equivalent of performing the calculation for a single technology), we get:

$$SI_t = \sum_{i=1}^{N_{ind}} \left(\int_{y=1}^{N_{years}} \sum_{j=1}^{N_{pi}} \frac{P_j - \min(P_j)}{\max(P_j) - \min(P_j)} * wp_{i,j} \right) * w_i \quad (47)$$

That indeed, is the sustainability score for a single technology. By neglecting the integral, considering only the yearly value of the sustainability score:

$$SI_{t,y} = \sum_{i=1}^{N_{ind}} \left(\sum_{j=1}^{N_{pi}} \frac{P_j - \min(P_j)}{\max(P_j) - \min(P_j)} * wp_{i,j} \right) * w_i = TechScore_{t,y} \quad (48)$$

This really looks like a sustainability score parameter related to each technology, and the final sustainability score will be calculated for each year as:

$$SI_y = \sum_{i=1}^{N_t} TechScore_{i,y} * AS_{i,y} \quad (49)$$

By doing this we have converted the initial evaluation method to an expression very similar to the Equation 40 where we have a fixed parameter multiplied for a variable.

In order to solve also the second issue related to the maximization/minimization problem, the sustainability score has been translated into an impact score by reversing the score, now the sustainability concept is reversed, creating an ImpactScore which is exactly is opposite. In this case, the yearly impact score will be calculated as:

$$ImpactScore_y = \sum_{i=1}^{N_t} TechScore_{i,y} * AS_{i,y} \quad (50)$$

In conclusion, starting from all the sets of parameters, a single score is defined for each technology following the same weighted sum process performed in the post processing phase. Then, is possible to obtain a scenario evaluation by applying this new technology-related parameter to a model decision variable like the activity (or its share) and calculating the sustainability score (or better the impact score, its opposite). This crucial step has been implemented in TEMOA, for the moment not as an extension of the objective function, but as an additional feature of the model which performs the sustainability assessment of the scenario once computed.

In order to pass from several sets of impact parameters to a unique impact value for each technology the abovementioned equations should be applied in an external framework, which must communicate with the core of the TEMOA model. A descriptive overview of the framework is available in Figure 28.

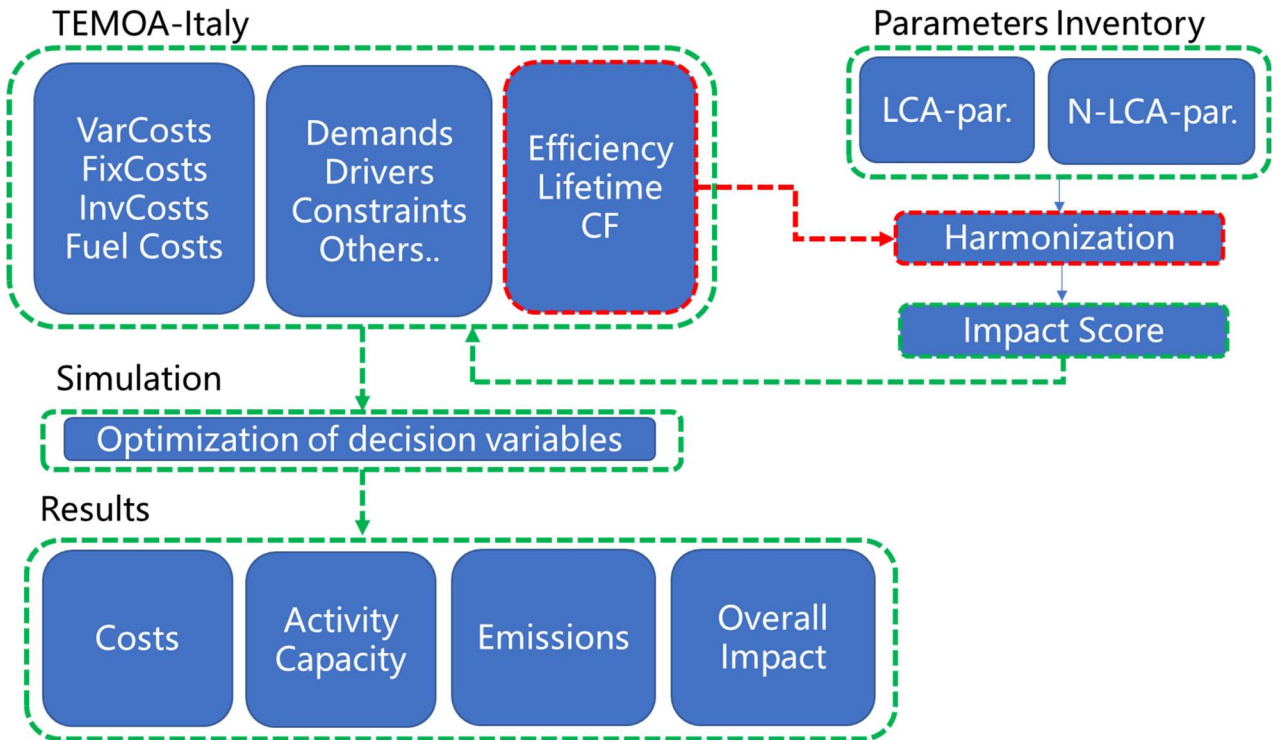


Figure 28. Framework for endogenous impact assessment.

In this framework data from TEMOA-Italy power sector are used to harmonize the LCA impact parameters. After that, the impact score database, in which a unique impact indicator is present for each technology and year, is sent to the model. Simulation, in this case not affected by the impact

score, select the optimal values for the decision variables in order to minimize the economic objective function. Finally, TEMOA provides results, including the overall impact score of the scenario calculated as in Equation 47. Is a simple integration of the postprocessing framework inside the model.

3.2 Simplified TEMOA-Italy

Now, let us enter in the core part of the sustainability paradigm integration. Till now, an operating framework has just been defined and the impact score parameter, associated to the technologies, has been inserted in the model making TEMOA able to calculate the final sustainability (or impact) score. In order to do whatever kind of multi-objective optimization integration, a model should be defined. In particular, starting from the TEMOA-Italy [23], a simplified version of the model has been created in order to allow a faster testing procedure. Given that the impact evaluation method is referred only to the power sector, only this one has been modelled. Industry, transport, residential and commercial sectors have just been modelled as electricity demand. In this way, there is no sectorial competition in satisfying the demand, since the only demand commodity is the electricity. If for example the transport sector was included, when considering the impact in the objective function the model could prefer the diesel vehicles with respect to the electric ones, in order to reduce the power sector activity and then reducing its impact, that will be finally included in the objective. In Figure 29 a model overview is shown.

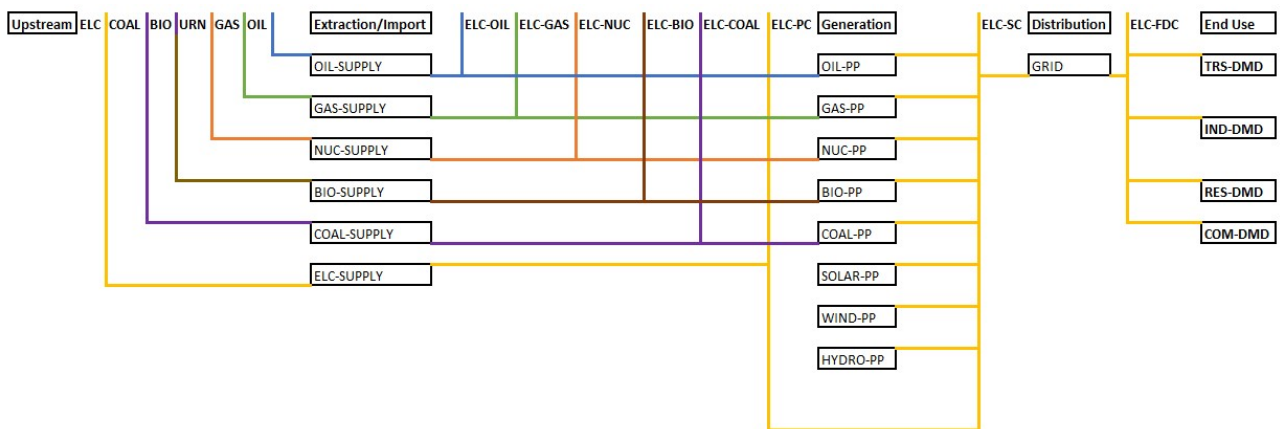


Figure 29. TEMOA-Italy simplified reference energy system.

As it can be noticed, the number of selected power plants is limited as it happens for the number of electricity demands considered. The reduced number of processes is not relevant since purpose of this model is to allow a rapid testing. Having few processes allow to rapidly replace wrong values and reduce the computational cost. These second motivation has a very high relevance when, in the next

part, the Pareto front of optimal solution will be plotted. In conclusion, the simplification introduced by this model are justified by its testing purpose.

Each process considered in the model came from the SubRES_NewTechs_2020 Upstream and Electricity sectors database of the EUROfusion TIMES Model [46]. Data of the model are reported in the following tables.

In Table 10 simplified TEMOA-Italy power sector is described through its technical parameters. With respect to the TIMES-Italy characterization present in Table 3, here we have both availability and capacity factor but, for TEMOA, they have the same meaning. Technology set is reduced to eight technologies, one for each plant typology, including the nuclear power plants. The inclusion of the nuclear power source may seem unrealistic for the Italian energy mix, but aim of this model is to demonstrate the application of a multi-objective function inside TEMOA and not to develop useful outcomes for policy-makers.

Table 10. TEMOA-Italy power sector.

ELC- Technology	SubRes Tech reference	LIFETIME	AF	CF	EFF
OIL-PP	EPLT: .G1.05.CON.OIL.Generic Dist Gen for Base Load.	30	0.85	-	0.37
GAS-PP	EPLT: .G1.05.ADV.NGA.Gas Comb Cycle.	30	0.95	-	0.58
NUC-PP	EPLT: .G1.05.ADV.NUC.Advanced Nuclear LWR.	40	0.8	-	0.35
BIO-PP	EPLT: .G1.05.CON.BIO.Sld Biomass Direct Combustion.	30	0.57	-	0.25
COAL-PP	EPLT: .G1.05.CON.COAL.IGCC.	30	0.8	-	0.47
SOLAR-PP	EPLT: .G1.03.CON.SOL.CEN.PVC.1	25	-	0.12	1
WIND-PP	EPLT: .G1.05.CON.WIN.CEN.Onshore.1	25	-	0.22	1
HYDRO-PP	EPLT: .G1.05.CON.HYD.Generic ROR Hydro.	45	-	0.5	1

In Table 11 the upstream sector technologies are present. They are fictitious technologies whose aim is to guarantee the supply of the power plants, but emissions data inside them are realistic given that they have been imported from the TIMES-Italy upstream sector.

Table 11. TEMOA-Italy upstream sector.

UPS- Technology	Input fuel	Input	Output fuel	Output	Capacity	CO2				
		to activity ratio		to activity ratio	to activity unit	emissions			activity	Unit
						A	F	CF		
OIL-SUPPLY	-	-	OIL	1	1	-	1	1	79.55	Kt/PJ
GAS-SUPPLY	-	-	GAS	1	1	-	1	1	56.05	Kt/PJ
NUC-SUPPLY	-	-	URN	1	1	-	1	1	3.6	Kt/PJ
BIO-SUPPLY	-	-	BIO	1	1	-	1	1	0.1	Kt/PJ
COAL-SUPPLY	-	-	COAL	1	1	-	1	1	101.2	Kt/PJ
ELC-SUPPLY	-	-	ELC	1	1	-	1	1	-	Kt/PJ

Finally, in Table Table 12, costs for all the technologies are reported. Units are different when referring to the power sector or the upstream one.

Table 12. TEMOA-Italy upstream and power sector costs.

UPS- Technology	2020			2050		
	INV, €/kW	VAROM, M€/PJ	FIXOM, €/kW	INV, €/kW	VAROM, M€/PJ	FIXOM, €/kW
OIL-SUPPLY	-	16.41	-	-	17.01	-
GAS-SUPPLY	-	6.34	-	-	8.34	-
NUC-SUPPLY	-	2.33	-	-	2.33	-
BIO-SUPPLY	-	4.39	-	-	6.4	-
COAL-SUPPLY	-	5.22	-	-	3.35	-
ELC-SUPPLY	-	6.9	-	-	7.78	-
ELC- Technology	2020			2050		
	INV, €/kW	VAROM, €/MWh	FIXOM, €/kW	INV, €/kW	VAROM, €/MWh	FIXOM, €/kW
OIL-PP	599.02	4.04	3.86	599.02	4.04	3.86
GAS-PP	880.00	0.65	20.00	676.92	-	-
NUC-PP	1500.00	0.06	60.00	1100.00	0.06	60.00
BIO-PP	2055.62	0.70	80.00	1603.38	0.70	80.00
COAL-PP	1800.00	0.30	54.49	1541.67	-	43.00
SOLAR-PP	1420.00	0.00	21.00	775.00	0.00	12.00
WIND-PP	1690.00	0.00	40.00	1235.00	-	30.00
HYDRO-PP	2500.00	1.11	30.00	2500.00	1.11	30.00

Repeating the steps followed in the ex-post analysis, once defined the technical parameters, the next step rely on the definition of the impact parameters. Since a wide set of parameters was already present due to the previous postprocessing phase, impact parameters for TEMOA-Italy technologies are selected considering the affinity of technologies with the previous tables. (From Table 4 to Table 8). Final parameters are reported in Table 13.

Table 13. TIMES-Italy impact parameters.

Technology Description	GWP	AP	EP	Mortality	Land use	Water Use	Decommissioning Cost	Noise Pollution	Health impact	TCRL	Reliability	Abundance	Diversification
OIL_PP	0.83	1100	110	36	0.4	1.94	31	90	0.19	14	75	50.7	18
GAS_PP	0.79	970	110	4	0.2	0.91	46	100	0.02	14	75	52.8	16
NUC_PP	0.04	46	119	0.04	0.15	2.77	1145	85	0	14	80	1000	135
BIO_PP	0.38	853	138	24	0.1	1.47	54	85	0.01	14	75	1000	135
COAL_PP	970	430	129	100	0.3	1.94	117	90	0.45	14	80	114	10
SOLAR_PP	0.1	528	44	0.44	10	0.34	57	60	0	13	22	1000	135
WIND_PP	0.01	61	4	0.15	1	0.08	51	105	0	11	17	1000	135
HYDRO_PP	0	0	0	1.4	10	1.7	290	97	0	14	50	1000	135

Following the path of the previous analysis after the parameters and their related indicators definition is necessary to set the weights. This opens an important topic related with the free-accessibility and the flexibility that this new version of TEMOA aim at reach. Indeed, the developed tool allows a user defined set of weights, both for the first order and the second order weights. This feature is really important since depending on the model type priorities may vary and a modeler could need a major focus on some aspects with respect to others.

Nevertheless, for this simplified version of the model, the set of weights has been left unchanged with respect to the previous phase on ex-post analysis. A recall of the previously used weights is available in Table 9.

Once defined the parameters and the weights all the ingredients necessary at combining the impact score with the model objective function are present. Indeed, the impact module of TEMOA takes in

input the impacts and the power sector, harmonizing the LCA data, normalizing everything and creating as output one impact score defined for each technology and year. After following these steps, the impact score is close to a variable cost or an emission factor, a simple parameter related to a technology which has to be multiplied for the activity of the plant. In Table 14 is possible to observe the final impact scores related to each technology.

Table 14. Impact score for TEMOA-Italy power sector.

Technology	Impact score
OIL_PP	0.451
GAS_PP	0.332
NUC_PP	0.229
BIO_PP	0.164
COAL_PP	0.529
SOLAR_PP	0.261
WIND_PP	0.296
HYDRO_PP	0.211

The last simplifying hypothesis is related to the activity and capacity constraints inside the model, in particular the model has been let free to choose the technologies it prefers, without imposing constraints on the already existing capacity or the planned installations. This because the focus is not in providing useful results in terms of energy scenarios analysis, but is more related to understanding how this sustainability parameter can drive the scenario generation.

Before proceeding in the core of the endogenous integration phase, a recap on the model attribute is necessary, in particular:

- TEMOA-Italy simplified is referred only to the upstream and power sector and the former is only functional to the latter.
- Upstream sector is modelled through six upstream technologies that supply electricity commodities
- Power sector is composed of eight electricity production technologies.
- Demand is only electric, a sectorial division of the demand is present, but is useless since all the sectors consumes the same commodity.

- Indicators, Parameters and weights are defined externally in the impact module of TEMOA, this last only send to the model a dataset containing the impact scores for each technology and year.
- Except for the base year, impact scores of LCA-parameters are defined through the harmonization process but, only in this version of the model, there is no evolution of the technological improvement drivers which cause constant parameters and then, the impact score is reduced to a vector defined for technologies but constant through the years.
- There are no constraints for the model decision variable like activity and capacity.

3.3 The Impact objective function

As it happens for Equation 40, the TEMOA objective function is only one of the many other expression created inside the model and solved by optimizing the choice of the decision variables. In particular, a simplified representation of these expression, which exclude the role of parameters like the global discount rate can be represented by:

$$\begin{aligned}
 TotalCost(Activity, Capacity) & \quad (51) \\
 &= InvCost * Capacity \\
 &+ (VarCost + FuelCost + FixedCost) * Activity
 \end{aligned}$$

Where, according to the TEMOA documentation [21], the activity decision variable is defined as the sum of the process output, determined by this equation:

$$Activity_{process} = \sum FlowOut_{process} \quad (52)$$

Capacity is the total size of installation required to meet all of that process' demands. In TEMOA, activity and capacity are related to a constraint that impose the installed capacity to be able to meet the activity demand. In mathematic terms it means that:

$$(coefficients) * Capacity_{process} = Activity_{process} = \sum FlowOut_{process} \quad (53)$$

Is not necessary to enter in the details for the coefficients since it is not relevant for our analysis. Aim of this TEMOA original objective function description is to understand the general structure that should be replicated in order to implement the impact objective function. By recalling Equation 48 with the considerations done in Equation 49 and Equation 50, is possible to highlight that in general,

the objective function is composed by parameters (the costs voices) and the FlowOut model decision variable.

This very general structure is the basis for the next implementation of the ImpactScore as a component of the objective function. Indeed, in this simplified version of the model the only output from the processes we consider relevant for the impact assessment (the power sector ones) is the electricity. This consideration is really important since in the final formulation of the impact score inside TEMOA the *FlowOut* variable will substitute the *ActivityShare* one that was present in Equation 47:

$$ImpactScore_y = \sum_{i=1}^{N_t} TechScore_{i,y} * AS_{i,y} \quad (54)$$

In this case, given that the sectorial competition is not present thanks to the simplified version of the model, there is no difference in using the activity or its share, because TEMOA is forced to satisfy all the demand with the Activity (or FlowOut) coming from the power sector processes. A future updated version of the model whose aim is to assess the impact of all the sector will require a specific module able to calculate the share of a technology in its sector. Nevertheless, in this way we get a new formulation of the ImpactScore as:

$$ImpactScore_y = \sum_{i=1}^{N_t} TechScore_{i,y} * FlowOut_{i,y} \quad (55)$$

Always remember that the terms process and technology are interchangeable in this analysis.

Referring to Equation 52 is possible to notice how the actual formulation of the ImpactScore looks really similar to the model objective function. The main difference relies in the term TechScore that can be seen as a “impact cost” for the single technologies as it happens for the cost voices, but not expresses in monetary units. As the different costs, the impact parameter is of “The lower the better” kind and this means that: If the ImpactScore is implemented as objective function, its minimization will correspond to an increase of the sustainability of the scenario, because minimizing the negative impacts of the power sector means increasing the benefits in terms of sustainability. Also, notice that the ImpactScore is defined annually, and there is a reason behind that. Indeed, in TEMOA the cost function is not optimized as a unique value for all the scenario duration, instead, the optimization process is performed annually. Indeed, the overall impact score calculation with the integral average theorem is performed in TEMOA just for output purpose but, for the optimization, only the annual

value calculation is required. The implementation of the sustainability paradigm inside the model is performed in two steps. The first and the easiest one refers only to the direct implementation of the ImpactScore inside the objective function neglecting the economic component. This will bring to a unique scenario evolution.

After that, sustainability and economic optimization paradigms are implemented in the same objective function, creating a multi-objective optimization problem. This part will lead to several scenarios generation and then, to the pareto front of the possible solutions.

3.4 First step: Sustainability-oriented optimization

Once implemented the sustainability paradigm calculation through the impact score formula, the economic-oriented objective function is substituted by the impact-oriented one. Inside the model Equation 48 is substituted by Equation 51. Since there is a single objective, a single scenario is generated. By referring to Table 14 and to Equation 51, it is possible to notice that the TechScore parameters are the only voices that are present in the equation and they are related to the FlowOut variable. In practice, it is like there is a single “cost” for each technology which is associated to the activity of this last. It is easy to understand that, if the model is left free to choose the technologies it prefers, it will select the less impacting technology. In this case the biomass power plant. These may seem a very stupid result but, if the simulation is run obtaining a one hundred percent biomass share scenario, there is the confirmation that the model correctly read and process the new objective function which has been implemented. Indeed, aim of this first test is just to check the correctness of the methodology implemented. This discussion is also confirmed by Figure 30.

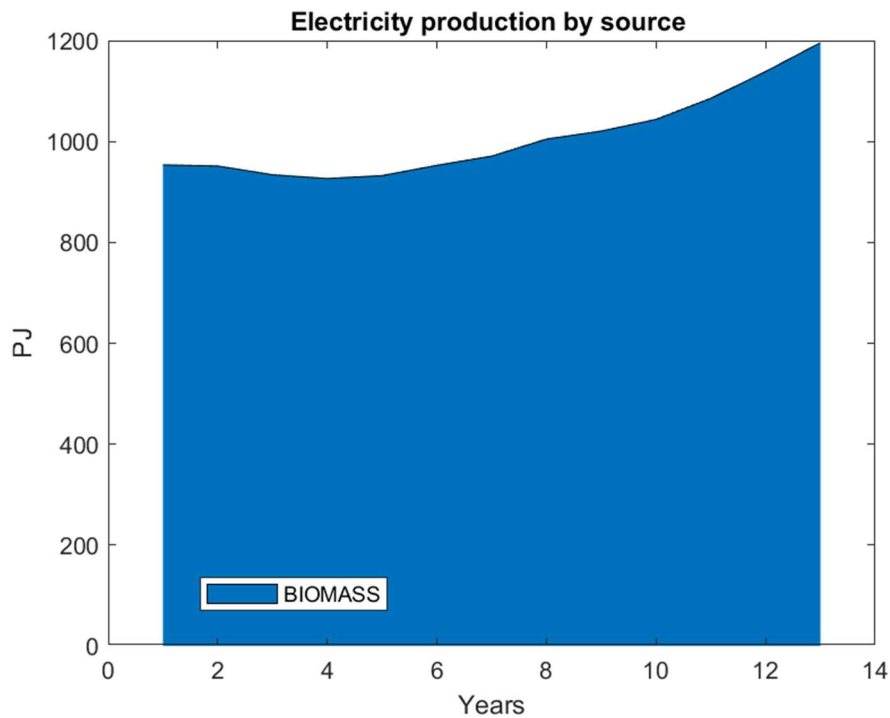


Figure 30. TEMOA-Italy energy mix with impact objective function only.

3.5 Second step: Economic-Sustainability oriented optimization

In this last, but not least part of the work the two optimizations (the economic and the sustainability ones) are combined inside the same equation. The equation which contains the economic and the sustainability related terms will finally constitute the model objective function. For the moment, let us imagine the model objective function in a very general sense:

$$Objective = f(TotalCost, ImpactScore, coefficients) \quad (56)$$

Where TotalCost and ImpactScore are the terms related to the two different objectives studied before. The important concept behind Equation 53 is that the objective value obtained by solving the multi-objective function will be the sum of two values: one for the ImpactScore and one for the TotalCost but, these lasts are not the values that would be obtained thanks to their single optimization. This because, as it happens for most of the multi-objective optimization problems, there is a trade-off situation in which minimizing one component leads to a maximization of the other one, and vice versa. But a trade-off problem it is not an absolute condition.

Till now, two version of the model has been proposed. The canonical one, in which a single economic optimization is performed and the version developed in this work that provides a sustainability-oriented optimization. In order to establish if the sustainability-economic is a trade-off problem as described above, is possible to look at Figure 31. Is clearly visible how the two optimizations bring

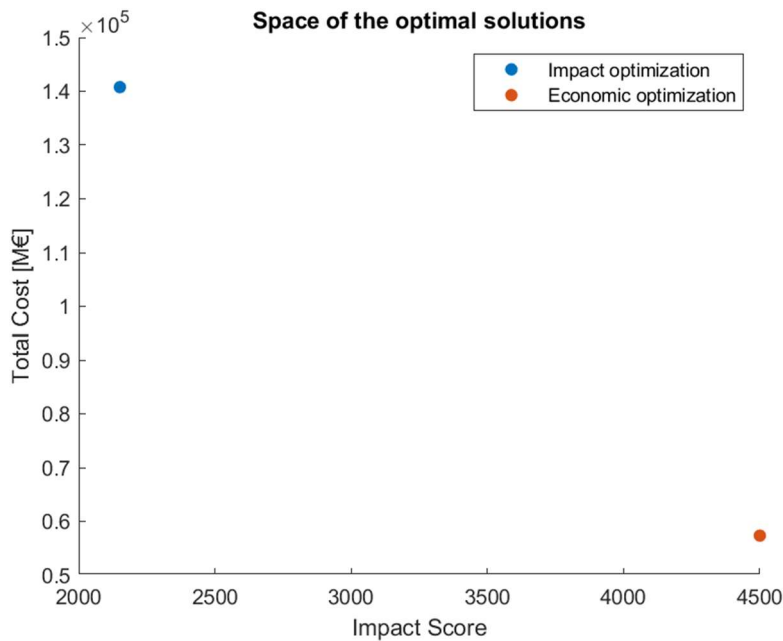


Figure 31. Differences between economic-oriented and sustainability-oriented optimizations.

to opposite solutions. On the x-axis the overall impact score is plotted while on the y-axis the total cost of the system.

When an economic-oriented optimization is performed the model totally neglect the sustainability problem and vice versa. Given that, when the model performs a single objective optimization the second objective (not considered in the equation) assumes very high values is possible to claim that the problem is of the trade-off type. This is not a necessary condition for all the multi-objective problems; indeed, we could have a beneficial effect of the second objective while optimizing only the first, but in general it doesn't happen. Especially in the energy field, the processes which are the worst from a sustainability point of view are cheap with respect to the ones that would guarantee a good sustainability performance. The title of Figure 31 is "Space of the optimal solutions" and indeed it represent the Impact-Cost couples at which the single optimizations may bring. In particular, if we recall Equation 53, writing it in a simplified form like:

$$z(x,y) = [f(x) + f(y)] \quad (57)$$

Where z is the value of the objective function and (x, y) the overall Impact-Cost couples, is easy to observe how this (x, y) couples represents the domain of the two variables objective function. In particular, the blue and red couples of Figure 31 are related to two possible solution of the domain but, since the objective function is a 2 variables one, the domain should be a 2-D in the x-y (or Impact-Cost) plane. Next step is to understand the shape of this domain or better, all the x-y couples that can bring to a feasible solution. The reason for this step is that, once known all the points of the domain, there will be some of them which could guarantee a lower (or minimized) value of the objective function with respect to the others, and we are interested in those couples.

3.6 Pareto front and epsilon method

Multi-objective optimization problems characterized by a trade-off dependence between the two objectives are well known issues in science. Let us take again the objective function formulation:

$$Objective = f(TotalCost, ImpactScore, coefficients) \quad (58)$$

And its general simplified form:

$$z(x,y) = [f(x) + f(y)] \quad (59)$$

As explained in the previous sections, both the TotalCost and the ImpactScore objectives are composed by fixed parameters and decision variables. In particular let us simplify the analysis

considering that the only variable involved is the *FlowOut* decision variable. This means that both $f(x)$ and $f(y)$ can be written as function of the same decision variable and then, also the objective will be function of the single decision variable *FlowOut*. Let us call the decision variable j , is possible to write:

$$z(j) = [f_1(j) + f_2(j)] \quad (60)$$

In fact, the two objectives *TotalCost* and *ImpactScore* are different functions of the decision variable j .

Is possible to introduce two definitions:

- A decision variable value j_1 DOMINATES j_2 if the solution associated to the former is no worse or strictly better to the solution associated to the latter in all the objectives that compose the final objective function, in this case:

$$f_1(j_1) \leq f_1(j_2) \quad (61)$$

$$f_2(j_1) \leq f_2(j_2) \quad (62)$$

- A decision variable j is called NON-DOMINATED or Pareto solution if there is no solution j' which can dominate j
- The set of non-dominated solutions of a multi-objective optimization problem is called Pareto front of optimal solutions

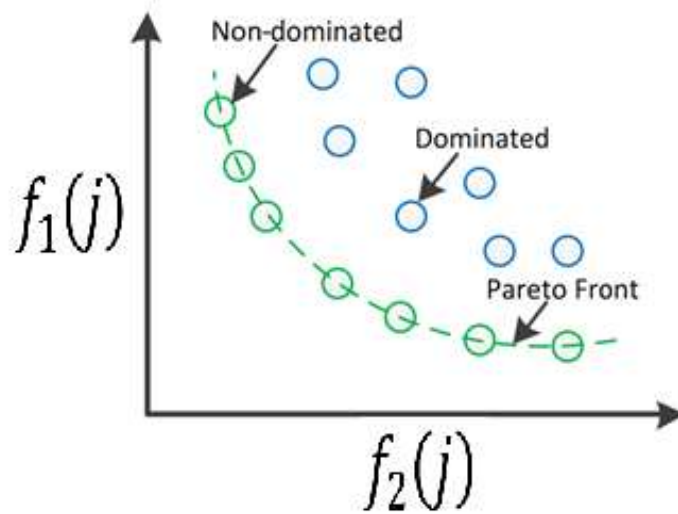


Figure 32. Pareto front of optimal solutions with dominated and non-dominated ones.

Following the above-mentioned definitions, in order to find the Pareto front of the sustainability-economic problem is necessary to calculate the non-dominated solutions of the problem. These last are the values of one objective that guarantees the minimum possible value of the other. In particular, for each ImpactScore (or TotalCost) value inside its domain, there are many TotalCost (or ImpactScore) values, but we are interested in the minimum one. Once known all the non-dominated solutions of the problem is possible to draw the Pareto-front. At this point it will be easier to formulate a proper objective function, because:

1. Pareto front is a set of solutions (Impact-Cost couples) , while objective function solution converges into a single couple. It must be guaranteed that final objective function solution falls on the Pareto line. Mathematically speaking, the solution point of the optimization, defined by the Impact-Cost couple, must belong to a point on the Pareto line.
2. Final objective function formulation should allow the prioritization of one of the two objectives depending on the user needs. Is important that the final prioritization covers different points on the Pareto front, because this implies control of the trade-off situation.

Summarizing, when dealing with a double-objective problem, finding the non-dominated solutions means optimizing one objective by keeping the second fixed. In this case, optimizing the TotalCost with fixed values of the ImpactScore that varies along its boundaries. This is also known as the ϵ -Constraint Method, which keeps just one of the objectives and translates the other objectives to constraints with user-specific values. Since TEMOA is an optimization model, by keeping only the cost objective function imposing the ImpactScore as a constrained varying between the boundaries found in Figure 31, for each value of the constraint it will find the optimal cost which is also the non-dominated solution. This procedure has been applied by manually inserting different values of the ImpactScore constraint between the interval 2151-4500.

As confirmed by Figure 33 the sustainability-economic problem creates a canonical Pareto front and this is due to the trade-off nature of the problem.

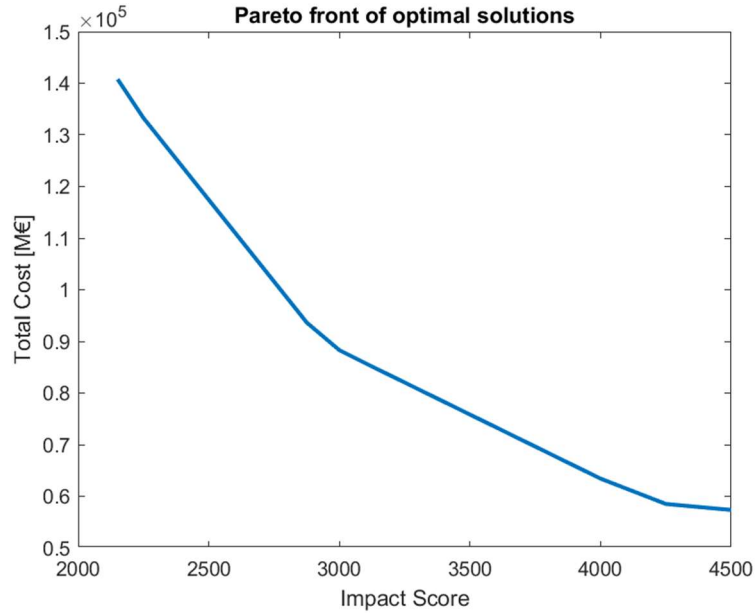


Figure 33. Pareto front of optimal solutions for the sustainability-economic in TEMOA-Italy simplified.

Selecting high values for ImpactScore allows lower costs, and vice versa. The plot has been obtained by interpolating the impact-cost points coming from several simulations, that is why the line is scattered. The Pareto front calculation is extremely important since it represents all the non-dominated impact-cost couples that constitutes the real domain of the objective function. Indeed, points below the Pareto line are unfeasible solutions, while the one which stays above are neglected by the model, because its final solution already falls on the blue Pareto line and is more optimized. In the next section it will be clear how the knowledge of this line is fundamental to test “a priori” several objective function formulations without inserting it directly inside the model, saving a non-negligible amount of time. Furthermore, is important to highlight that each point on the pareto represents a different energy system scenario, characterized by different activity and capacity of installed plants. Indeed, ImpactScore and TotalCost are connected to the FlowOut decision variable that finally determines the activity and the capacity.

In Figure 34 cumulative activity by source for each scenario obtained varying the *ImpactScore* constraint is present. Fourteen equally spaced points has been selected inside the *ImpactScore* domain

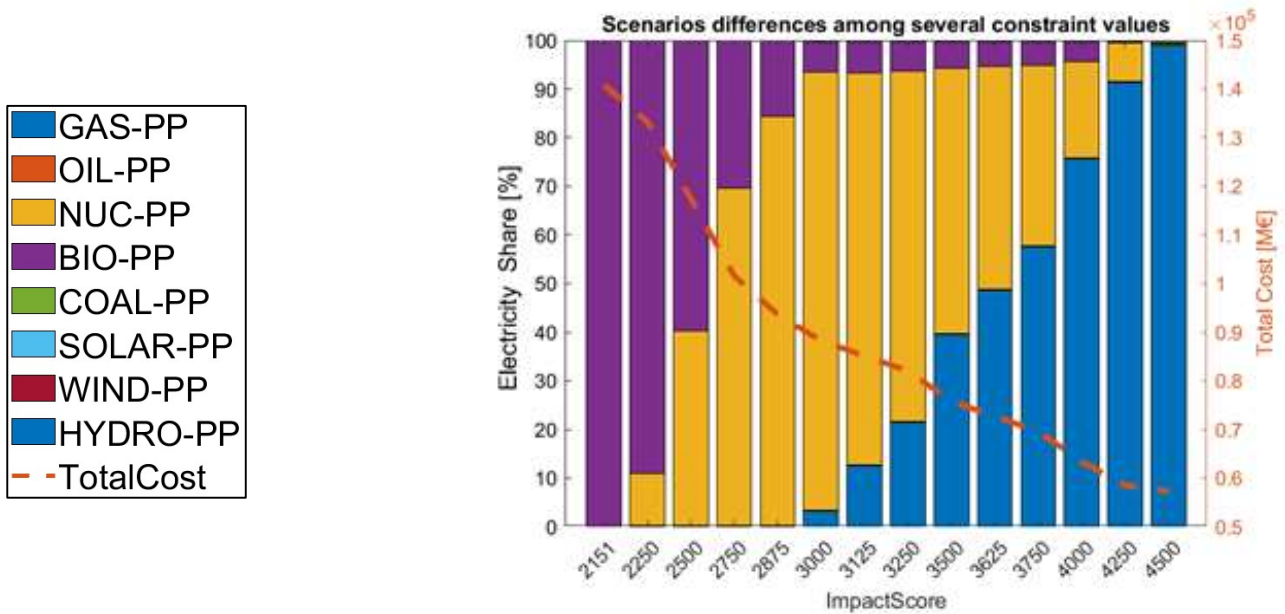


Figure 34. TEMOA-Italy simplified scenarios differences while varying the *ImpactScore* constraints.

of variation. For all of these points a simulation has been performed obtaining different scenarios. Then, activity of power plants for all the years has been summed keeping the division for type of technology. Interest is in how the scenarios evolve by changing the *ImpactScore* constraints. Thanks to this equally spaced configuration is possible to see the gradual shift towards cheap and impacting technologies when increasing the value of the constraint. This result is quite intuitive since the number of technologies is limited to eight. Indeed, is simply necessary to substitute a little share of a cheap and emitting technology with a costly and more sustainable one in order to do a little step on the impact. More interesting would be the case in which lots of technologies are present. Indeed, in this last situation a little reduction of the *ImpactScore* constraint may bring to a different energy scenario.

3.7 Multi-Objective function: implementation and results

Till this point, the multi-objective function has never been mentioned if not in a very simplified form as shown in this equation:

$$Objective = f(TotalCost, ImpactScore, coefficients) \quad (63)$$

Indeed, the final objective function formulation is not known a priori, but its final form strongly depends on the nature of the problem (that in this case is of a trade-off type) and is also related to the needs of the user with respect to the problem. Indeed, the objective function is usually a fixed type formulation which, once optimized, converges into a single system configuration. Given that in this analysis there is a trade-off situation, a TEMOA user may be interested in creating energy scenarios combining the sustainability and the economic aspects also giving different relevance at the two aspects. In order to perform a “ad-hoc” optimization is necessary to define an objective function with a flexible structure that allows first of all, to put on the same plane different amounts and also, to give at the two objectives a different relevance (the economic and the sustainability ones) inside the final objective function formulation.

This desired form of the objective function is made possible by a common method used in multi objective optimization problems, the weighted sum method [47].

In general, the weighted sum approach transforms Equation 53 in this general formulation:

$$Objective = \alpha * TotalCost^n + \beta * ImpactScore^n \quad (64)$$

Where the two coefficients are the weights of the two objectives:

$$\alpha + \beta = 1 \text{ and } \alpha, \beta \in (0,1) \quad (65)$$

Referring to Equation 64, is possible to observe a problem related to the use of this function. By looking at Figure 33 is possible to observe that the *TotalCost* has a magnitude of $1e5$, while the *ImpactScore* is limited at $1e3$. Even if the weight assigned at the *ImpactScore* is 0.9, the *TotalCost*, thanks to its magnitude, will have an higher share in the final value of the objective function and the model would be stimulated in reducing the cost component independently to the weights assigned. Moreover, even if the two objectives are at the same order of magnitude, there is still a problem

related to the range of variation. Imagine the case of having two objectives in the order of $1e6$, but the first one varies in a range between 1 to 9 while the second in the interval 1.5-2. Even if a larger weight is assigned to the component with a thin range, the model would enhance the component with a larger window of variation, again because a 10% reduction of this last will give a major contribution with respect to a 90% reduction of the second. Is then necessary to calibrate one of the two components at the same order of magnitude and range of variation of the other in order to guarantee, at least in theory, a proper role of the weights.

The objective function is then re-formulated as:

$$Objective = \alpha * TotalCost^n + \beta * LevImpactScore^n \quad (66)$$

Where the term *LevImpactScore* is calculated through the equation:

$$\frac{ImpactScore - \min(ImpactScore)}{\max(ImpactScore) - \min(ImpactScore)} = \frac{LevImpactScore - \min(TotalCost)}{\max(TotalCost) - \min(TotalCost)} \quad (67)$$

Is a sort of normalizing procedure but performed by bringing one component at the level of the other. Notice that in the above written equation the *ImpactScore* and the *LevImpactScore* terms are not known until the objective function is solved. The terms which are known “a priori” are the boundaries of the two objective function components, but the calculation of these last requires a calibration phase of the model by performing two separated single objective optimizations: an economic-oriented and a sustainability-oriented. In this case, the two single-objective optimizations are already performed and shown in Figure 31, since this data remains the same if the model data are unchanged.

Once finished the calibration process, there is still a term that miss, the exponent of the two components. Till now, at least in theory, different weights should result in different trade-off points on the Pareto front; however, in reality, the story is not the same. Different weights can lead to the same point or points very close to each other, consequently, the points are not uniformly distributed on the Pareto front. There is not a general methodology to avoid this issue and there is still active research on that [47], but the exponent choice can give a significant contribution in improving the Pareto front coverage when changing the weights.

Let us take the case in which the exponent is equal to 1. The objective function is now:

$$Objective = \alpha * TotalCost + \beta * LevImpactScore \quad (68)$$

Or, referring to a single coefficient:

$$Objective = \alpha * TotalCost + (1 - \alpha) * LevImpactScore \quad (69)$$

With this last version of the objective function several simulations has been made by considering different values of α going from 0 (only sustainability optimization) to 1 (only economic optimization). A similar visualization as the one proposed in Figure 34 is shown. Cumulative power plants activity share is plotted for scenarios coming out from the solutions calculated with different values of alpha.

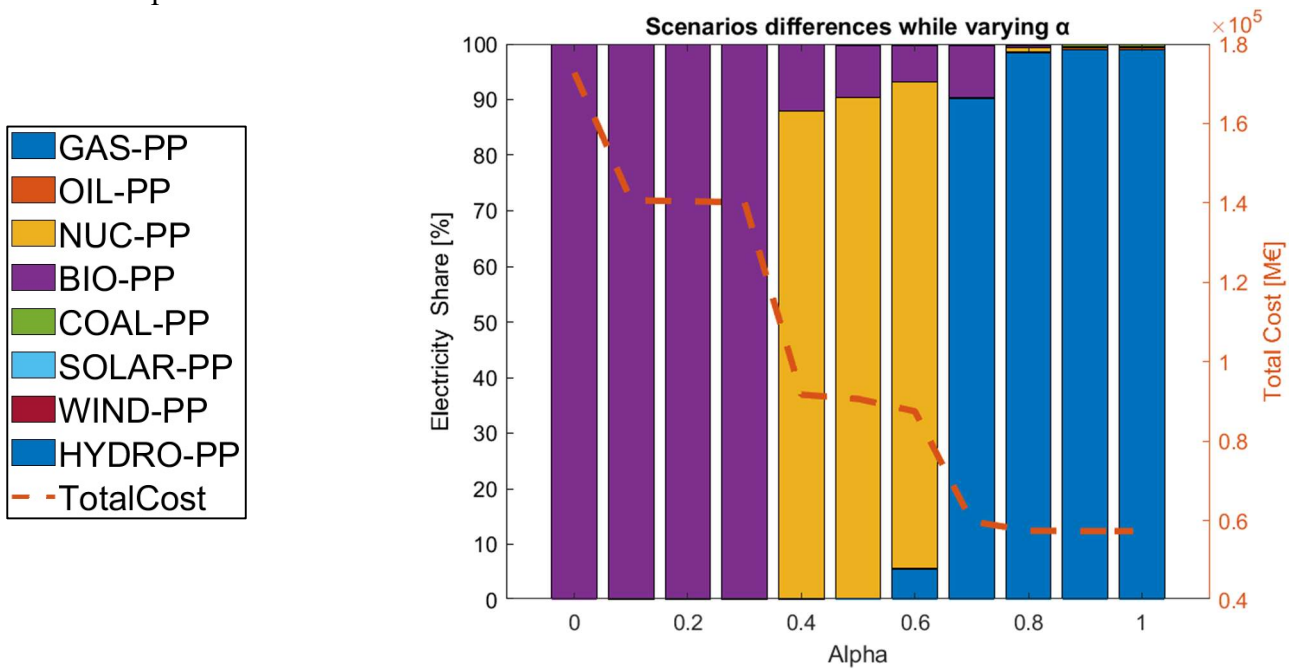


Figure 35. TEMOA-Italy simplified scenarios differences while varying the α value-first test.

Is easy to notice the differences that Figure 35 and Figure 34 presents. In particular, if in the ε -method the technology shift is gradually obtained, here the solution of the model jumps from a configuration to another one, which is totally different from the previous. Before making any other comparison between the two figures is important to make a premise: A different imposed ImpactScore with the ε -method means imposing a different solution, because we are forcing the solution to fall on another cost-impact non dominated solution. Imposing α is not the same thing, changing its value does not guarantee that the solution points will change. Indeed, the ε -method forces a solution of the problem while the weighted sum just changes the objective function formulation, but the final solution (the minimum of the objective function) can fall on the same impact-cost couple. This discussion is also confirmed by Figure 36.

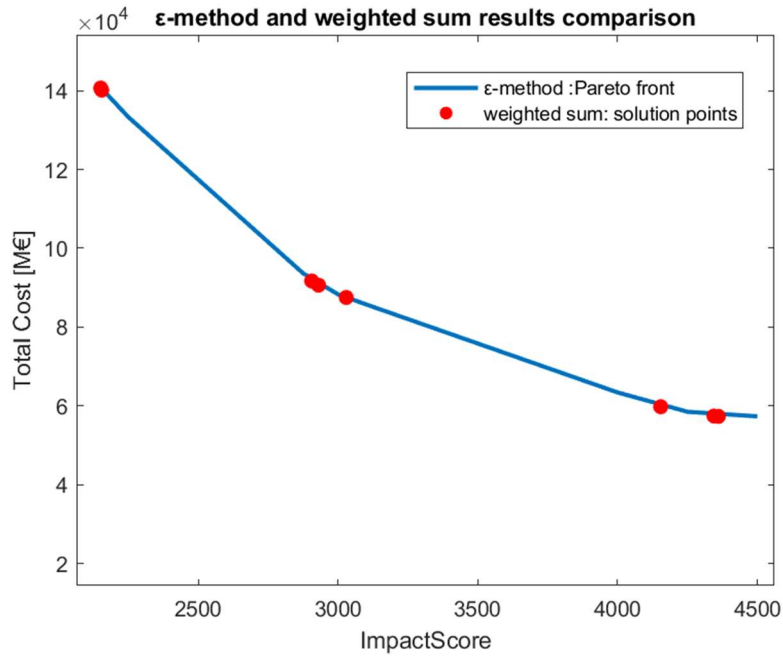


Figure 36. Differences between the ϵ -method and weighted sum approaches.

The red points are the solutions of the objective function for different values of α . As visible, even if α varies uniformly in the range 0-1 with a finite step variation of 0.1, the impact-cost couples in which the solutions fall are concentrated in three areas of the plot and, inside the single area, they are very close to each other. This situation is very problematic since the role of the α coefficient, which serves as a “trade-off” choice parameter that allows the user to prioritize/penalize one of the two components, is thwarted by this issue. In particular, there are situations in which varying α doesn’t imply a change in the final solution, even if the objective function is different. This is because, as already explained, different objective functions can converge around the same minimum. A detailed representation of the problematic is well described by Figure 37.

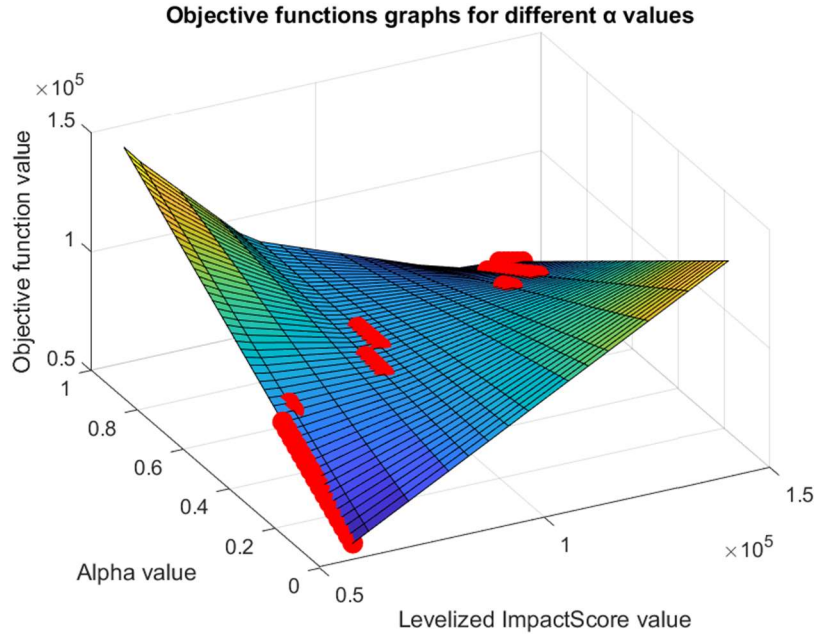


Figure 37. Minimum points for different objective functions graphs obtained by varying α

The above representation has been obtained in a postprocessing way, starting from the Pareto front. Indeed, once obtained the set of non-dominated solutions with the ε -method there is no difference in working with objective function directly inside the model or an in ex-post analysis. The model defines simply the set of the optimal points that constitutes the Pareto line (domain of the objective function, whatever is its form), and the objective function as already explained, is a single point of the Pareto. Once known the domain of a function, is possible to play with this last outside the model. This simplifies the process allowing a faster analysis.

Coming back to Figure 37, the lines parallel to the sheet are the objective function graphs obtained by varying α in its range of variation. Indeed, is possible to see that when α is low (impact prioritization) the solution converges to low levelized ImpactScore, and vice versa. The red points are the minimum of each objective function. This plot aims at reproducing the behavior of the model, that once known the objective function find the minimum impact-cost (or levelized ImpactScore referring to Equation 66) couple of this last. The position of the red points, calculated for more than one hundred α values, confirms the above-mentioned issue of coverage of the Pareto front. What the picture suggests is a threshold problem. Till a limit value of α the model keeps considering a certain solution the best. Then, from the previous limit to another one, the solutions for different α keep falling on the same point (or very close points). This phenomenon happens three times in this specific case, and it is localized in the bottom, top and medium part of the solutions space.

All these considerations have been done in a postprocessing environment but, in order to test what experimentally theorized, the TEMOA-Italy simplified has been tested with more than 50 objective functions considering different α values, especially in those points which are closer to a “jump” of the solution.

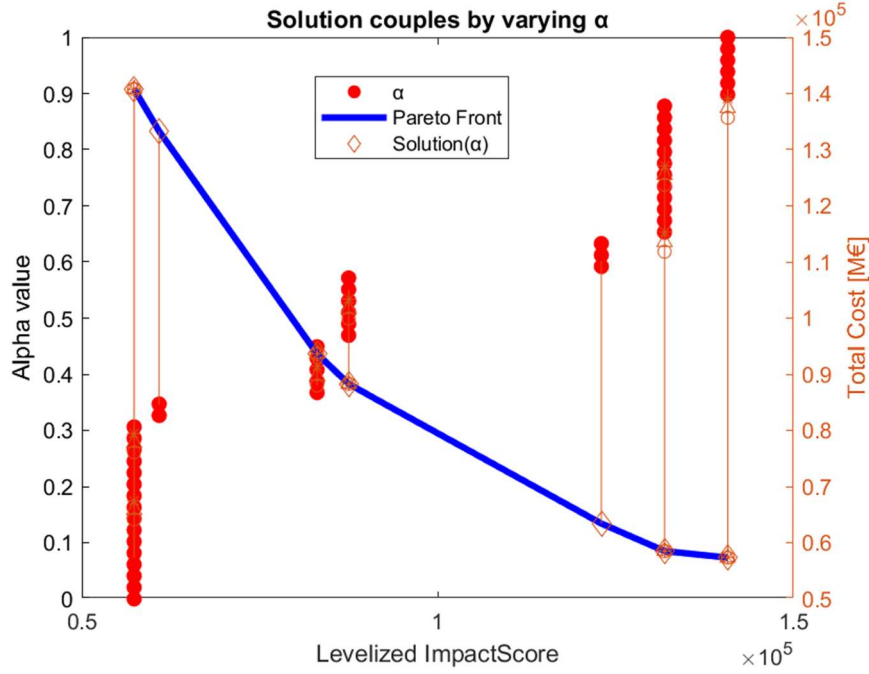


Figure 38. Solution of several objective functions obtained by varying α , related to α value.

Result of the abovementioned α - variation optimization process in TEMOA-Italy simplified is shown in Figure 38. This plot relates the values of α (indicated by the red dots) with the solution that the objective function in which the respective α value is inserted, provides. Is clear that, even inside the model, the threshold process before theorized happens. From one side, this is a good confirmation of what has been just a hypothesis till this point, but somehow, this issue has to be solved. One approach is to change the objective function, always using a weighted sum formulation, but with a quadratic exponent of the two components:

$$Objective = \alpha * TotalCost^2 + (1 - \alpha) * LevImpactScore^2 \quad (70)$$

With this new formulation is possible to repeat the same considerations done for Equation 66. Starting from the scenario cumulative electricity share evolution while varying α , is possible to observe in Figure 39

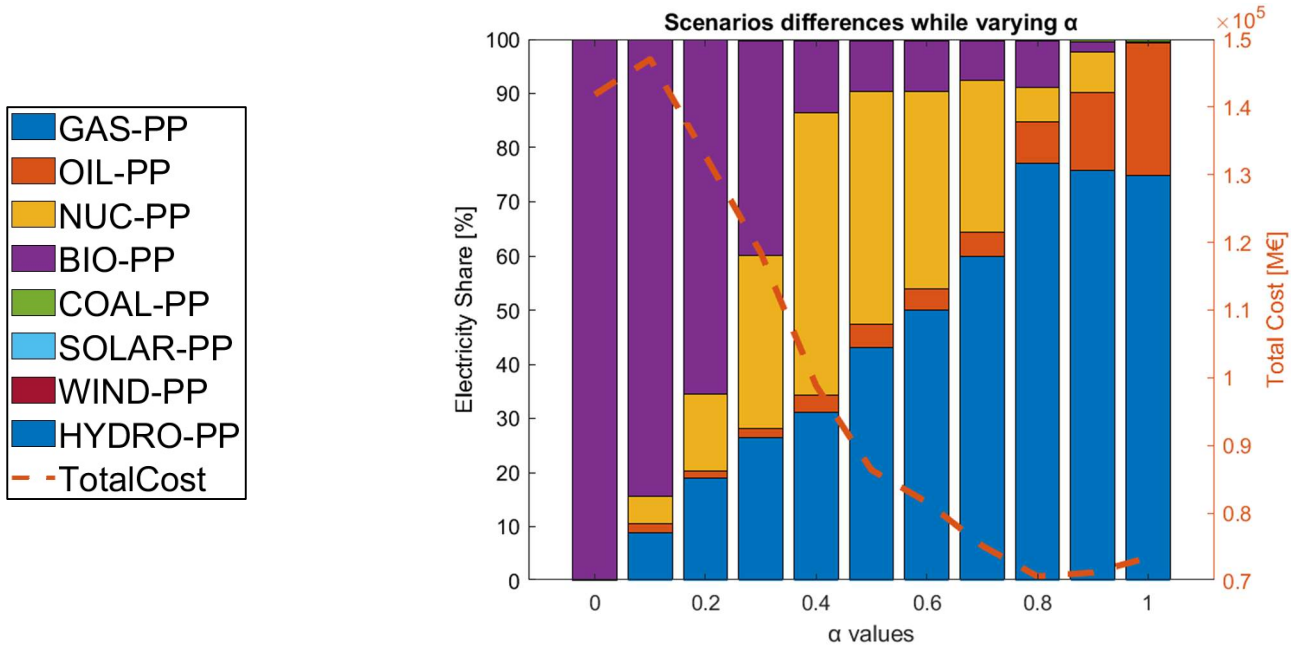


Figure 39. TEMOA-Italy simplified scenarios differences while varying the α value-second test.

that the technological shift is smoother with respect to the previous case and also, there is a new technology in the electricity mix which is not originally present in the set of dominated solutions highlighted by Figure 34. So, there is a good aspect related to the Pareto coverage but an ambiguous fact due to the presence of the oil power plant in the energy mix, which is different from the previous examined Pareto solutions. Concerning the coverage of the Pareto front, is possible to repeat the same ex-post analysis done before to the quadratic objective function, by testing what happen at the minimum location (or better, at the objective function solution location) when trying different values of α inside the objective function formulation.

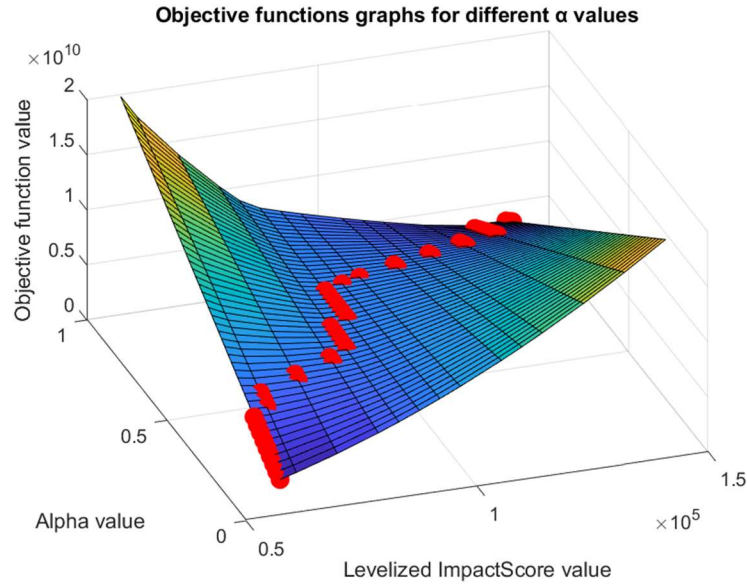


Figure 40. Minimum points for different quadratic objective functions graphs obtained by varying α .

With a quadratic objective function it is possible to observe how the issue is not totally solved, but its behavior is improved. Now there is a wider coverage of the impact-cost solution couples, even if three cumulative impact-cost couples present a higher number of α values that determines the solution couple. Another intuitive visualization of the improvements obtained with a quadratic objective function is shown in Figure 41. Now the distribution of the optimal solution points is really improved at least in theory, since Figure 41 and Figure 40 has been obtained by externally computing the objective function starting from the domain of the model solutions.

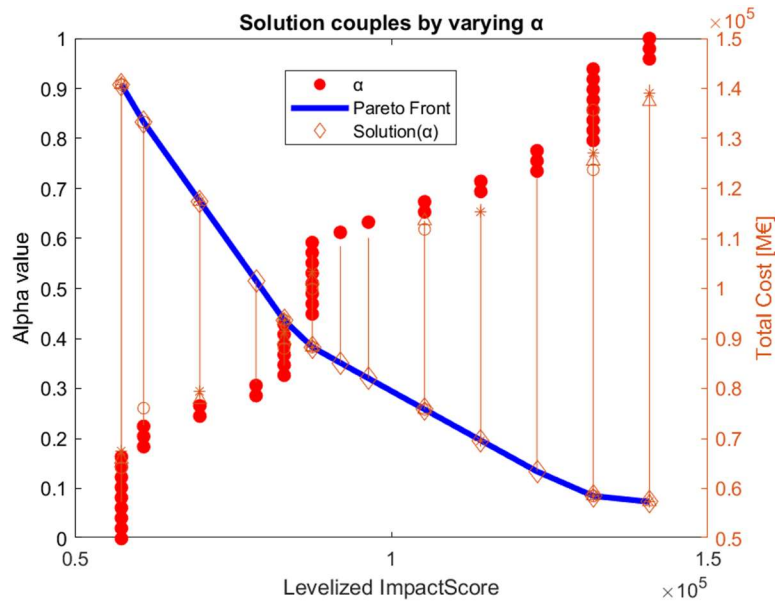


Figure 41. Solution of several quadratic objective functions obtained by varying α , related to α value.

When repeating the analysis inside the model, by testing what happen at the solution with quadratic objective function characterized by different values of α , is clarified why in Figure 39 there is oil in the electricity production mix and why the TotalCost has an inversion of the trend at the extreme points of the plot. Let us focus on Figure 42 where a comparison is present between the models with a linear and quadratic objective functions when varying α between zero and one.

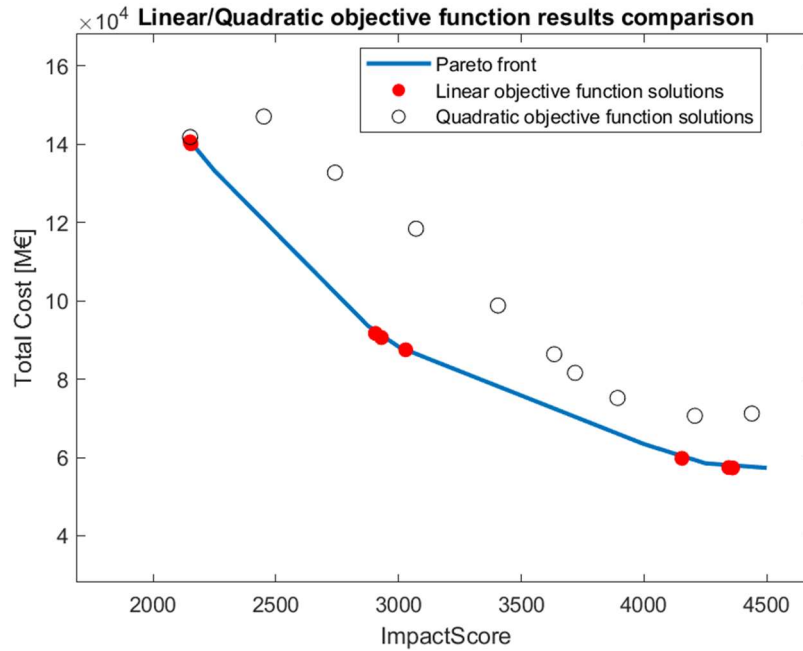


Figure 42. Differences between solutions of linear and quadratic objective functions.

Is clearly visible from the plot, that when a quadratic objective function is used a better coverage of the Pareto front is guaranteed, especially if compared with a linear type. In this way is possible, by varying α to obtain different trade-off choices of the problem, and this is a good goal. The problem related to the quadratic objective function rely in the solution algorithm, in particular the one used to solve the linear formulation is not efficient in solving also the quadratic one. Indeed, the solution points of the quadratic type are of course well distributed in the space, but at a higher cost. These means that the model is unable to get a non-dominated solution when solving a quadratic expression. Indeed, the white points still require a cost optimization and for this reason they are dominated solution, because on the Pareto a solution with the same impact and a lower cost exists. Is then necessary to change the solution algorithm to reduce the cost of the quadratic solutions.

Chapter 4: Conclusions and perspective

In order to conclude this analysis, is necessary to remark the achieved objectives, highlighting the current limitations that will constitutes future improvements. The first half of this work has been devoted to the building of a flexible framework able to translate the different aspects and parameters that quantifies the sustainability into a single numerical value. Results applied to TIMES-Italy scenarios have shown that is possible to combine low carbon scenarios with sustainability goals since, in general, the fuel combustion technologies are the ones which presents higher emissions and also, a lower sustainability score. This is not valid for the biomass and nuclear power plants, for which the impacts strongly depend on the type of power plants considered. These aspect opens at a first limitation of this analysis. Indeed, data for impact parameters are not defined for each technology, especially the LCA type. An extension of the LCA databases to a wider set of technologies will be beneficial for these kinds of analysis since it would give a cleared direction towards the best technological choices, even inside the same power plants category.

Concerning the first part methodology, a further extension of the sustainability assessment framework capability is necessary. In particular, the developed framework has been thought for an integration inside the model and then, it is limited from the aspects which can be captured. Postprocessing tools can be very useful in evaluating the consequences related to scenarios with a higher degree of electrification, also involving aspects as infrastructure requirements, resource consumption and storage requirements. In general, all the aspects that are difficult to be modelled and related to decision variables can be studied in an ex-post analysis but the latter requires an extension of the existing framework. Furthermore, even if the developed framework is already flexible, work is needed in order to create an easy interface in which user can insert technologies, scenarios and parameters. The latter aspect is required since the desire is to have an open-science approach.

Moving to the second phase of this work, related to the endogenous integration, opens at several considerations. The target of changing the model paradigm thanks to the integration of a sustainability index as part of the model decision variables has been achieved. These steps have shown interesting results despite the simple model taken as a case study, in particular:

- In the Pareto front, starting from the least cost solutions, three macro-trends can be individuated by moving to the least impact solution. The individuated trends are characterized by an increase of the slope, sign that a little increase of the sustainability performance is possible without penalizing too much the costs. Clearly, when moving to high levels of

impact, the marginal cost of the sustainability increase and this is particularly evident in the last phase of the Pareto moving from the bottom to the top.

- The developed framework can have a double utility. It can be used for long term energy scenario development as done in this work, but also in the short-term energy planning. Due to its flexible formulation is easy to be implemented in the objective function of models that aim at satisfying the near-term demand combining the generation plants, as the dispatchable-models. Also, thanks to the framework flexibility, is possible to integrate different parameters to better adapt the framework at the regional context under evaluation.
- Inserting sustainability parameters inside an optimization model does not bring to results that are “far from reality” from the point of view of the technology considered. The message behind this last consideration is very positive since it tells us that, with a smart use of the available technologies is possible to increase the sustainability level of the energy system without drastically changing them.

As much as the target reached, the possibilities of improvements raised up by this work are:

- The creation of specific modules inside TEMOA whose aim is to calculate a sustainability parameter, no more related to the single technology but to the overall electric system. These may be very beneficial when calculating the diversification, the import dependence and in general all the security parameters related to the system configuration and not to the single technology.
- The extension of the impact assessment at the other sector, in order to let the model free to decide how to satisfy a certain service demand, accounting for the sectorial competition in terms of sustainability. The sectorial extension may give interesting results especially in the transport and in the industry sector, where is possible to satisfy the demand with different commodities.
- The necessity of a further step in terms of optimization. First of all, the weighted average which is the basis for the impact assessment as developed is a deterministic method. A deterministic method assumes no uncertainty about the weights assigned and the change of preference that can happen in future. Advanced method are available for that, as the utility one. Indeed, the utility method considers uncertainty in the weight assigned at each parameter, which is a more realistic method because there is always some degree of uncertainty. The second important step is to move to a real multi-objective optimization solution. Weighted sum is still a single objective function. In a multi-layered problem like the sustainability is necessary to create different dimensions of the problem that are finally optimized in parallel.

This extension is necessary if aim is to open the model at important energy related problem like the reliability-security of the grid and the water-energy-food nexus.

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