A Conceptual Framework for Comparing Alternative Commodities in the Energy Transition

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***Abstract*—The global emissions increase requires the adoption of proper countermeasures, aimed at tackling climate change. On the one hand, the transition towards a renewable-based energy sector is an undeferrable need, because of its important impact on the overall emissions balance. On the other hand, a single final use can be fed by more than one commodity, and their coexistence/competition paves the way to the development of a multi-commodity energy system, enabling the implementation of the so-called "cross-sector integration". In this paper, we propose a conceptual framework for the comparative assessment of the various energy commodity chains, aimed at defining the preferrable ones for residential and transport uses. The evaluation of their overall performance is carried out determining the quantity and the quality of the involved commodities, by adopting energy and exergy efficiency along the entire chain, provided that one unit of primary energy can supply one chain only. This straightforward assessment method is not constrained by any generation capacity and/or emission related targets and introduces a commodity-based evaluation framework, that differs from the already existing ones that adopt a technology-oriented approach.**

***Index Terms*—Energy Transition, Cross-sector coupling, Electrification, Hydrogen, Decarbonization, Energy mix**

I. Introduction

During the course of last years, the necessity to decarbonize the energy system has become more and more pressing. Climate change, most likely caused by human activities, requires immediate actions to not overcome the temperature increase of 1.5°C with respect to the pre-industrial era, as wished for in the Paris agreement [1], and also recalled by the recent UN Climate Change Conference (also known as '26th Conference of the Parties', COP26) in Glasgow (UK) [2]. Hence, the importance of Renewable Energy Sources (RES) increased, because they represent carbon-free energy sources. As a consequence, different countries invested and will invest on RES, to create a decarbonized electricity generation system. The European Union, although representing about 8% of the total worldwide emissions, aims to reach carbon neutrality by 2050, an ambitious target that implies the commitment to cut emissions at least of 55% by 2030 [3]. On the other side, the power output of all these resources is intermittent, and this poses new challenges in the operation of the power grid [4] and in coping with the needs of final uses. Moreover, about 80% of the world energy consumption [5] is presently not electrified, and its total electrification is considerably challenging, if not unfeasible (e.g., in the case of high-temperature process heat [6]). Considering that a single final use may be fed by more than one commodity, a multi-commodity energy system can be introduced as means to satisfy the different energy needs while decarbonising them [7]. However, this scenario must be carefully investigated to avoid a misestimation of the required amount of RES, transmission/distribution and/or storage infrastructure capacity for its actual implementation.

Trying to answer the above questions is not easy, as the choice of the optimal energy mix must adequately weigh three aspects, known as the energy trilemma: equity (in terms accessibility and affordability), environmental sustainability and energy security [9]. Nonetheless, the problem of finding the optimal primary energy mix was investigated in several works, also addressing different spatial scales. In [10] seven fundamental aspects to be considered whenever searching for the optimal energy mix were suggested. The optimization models implemented by the majority of the authors aim at finding the most cost-effective combination of primary energy sources, subject to constraints in terms of emissions of polluting gases, available budget and/or available land for the installation of new generation capacity. In [11] the renewable potential of the Grand Canary Island was analysed to find the optimal renewable generation mix, targeting the decarbonisation of the energy supply of the island by 2040. A model for the cost-optimal decarbonisation of the industrial, power, heating and transport sectors, aimed at finding the best combination among electricity, hydrogen, natural gas and synthetic methane, was developed in [12]. A similar study was carried out in [13], where evolutionary algorithms were applied in combination with a predictive control strategy, to find the least expensive mix of renewable generation and storage technologies. Some works focused on a particular final use: in [14] the authors developed a multicriteria analysis to find the best RES mix, capable of supporting the charge of electric vehicles. In [15] possible trajectories to decarbonise the British heat supply were analysed. Electrification and a decarbonised hydrogen supply were identified as two potential drivers of the future energy supply mix. An optimization model to define the best decarbonisation strategy of an oil refinery was carried out in [16]. In [17] a review and classification of existing bottom-up optimization models, according to four different criteria, was performed. In [7] the authors carried out an even more detailed analysis of existing energy systems optimization models, categorizing them according to their modelling approach and resolution, and technological detail. Most of the works reviewed by the authors share a common approach based on optimization models drawing on input datasets (generation and/or load profiles, fuel prices, meteorological data, techno-economic characteristics of technologies) and aimimg to minimize/maximize a particular objective function (usually the overall expenditure). The problem is then subject to several constraints, such as maximum GHG emissions and/or maximum share of renewables in the generation mix.

This paper presents a conceptual framework for the comparative assessment of the various energy commodity chains, aimed at defining the preferrable ones for residential and transport uses. The evaluation of the overall performance is carried out by evaluating energy and exergy efficiency along the entire chain, provided that one unit of primary energy can supply one chain only. This straightforward assessment determines the quantity and the quality of the involved commodities without any generation capacity and/or emission related constraints and introduces a commodity-based evaluation framework, that differs from the existing technology-oriented approaches. The reminder of this paper is the following one: Section II defines the commodity chains and the covered sectors; Section III introduces the application of the First and the Second Law of Thermodynamics to rank the different chains; Section IV shows the results, while the last section reports the final remarks and the future works.

II. The Commodity Chains

A. Introduction and definition

To properly define commodity chains, a prior distinction between primary commodities and primary energy sources is necessary. Primary commodities refer to the energy carriers that are directly harvested from natural resources. They may or may not coincide with the primary energy sources they are extracted from: for instance, oil and natural gas are both primary energy sources and primary commodities, whereas solar irradiation is the primary source from which the primary commodity electricity is produced. The concept of secondary commodities can be introduced: they are obtained by converting primary commodities in ad-hoc devices and/or facilities. For example, hydrogen obtained by electrolysis can be regarded as a secondary commodity, as well as electricity generated in thermal power plants. On this basis, a commodity chain is defined as the representation of the energy flow, from primary sources to final uses, by including also its use and/or manipulation in intermediate stages, such as conversion, transmission, storage, distribution, and transformation into appliances and devices providing the final energy service. A comprehensive view of what is meant by commodity chains, together with the holistic representation of a multicommodity energy system, is displayed in Fig. 1.

Energy commodity chains generally consist of six stages:

- *Primary Energy Sources*: renewables (solar, wind, and hydropower, marine and ocean energy, and biomass) or non-renewables (natural gas and uranium ores).[1]
- *Conversion*: the process of transforming a primary energy source into a primary energy commodity (or from a primary to a secondary commodity).
- *Storage*: the stockpiling of a commodity for its future use (i.e., time decoupling between the generation production and the use).
- *Transmission/Transport*: the movement of large amounts of energy across long distances (e.g. UHV electric lines or transcontinental gas ducts); hence, it guarantees the space decoupling between generation and use.
- *Distribution*: the infrastructure that moves the energy commodities in a limited geographical area, and lying between the transmission infrastructure and the final uses.
- *Transformation*: the process of adopting ad-hoc devices (boilers, heat pumps, fuel cells, internal combustion engines, reforming furnace, etc.) to produce a useful effect exploiting the energy content of the inlet commodities at the consumer level.

Specific chains may either include all the above stages or only a subset; moreover, their reciprocal order might be different in the actual implementation.

B. Covered sectors

We classified final uses into three main sectors, according to the energy service they provide to final users:

- Residential, including space heating and cooling, domestic hot water (DHW) production, lighting, and cooking.
- Transport, consisting of freight and passengers' mobility.
- Industrial, including ancillary equipment, low-, medium-, and high-temperature processes, and refrigeration.

This work specifically focuses on *space heating* applications in the residential sector, and technologies for the propulsion of *light duty vehicles* in the transport sector.

III. Quantitative Evaluation of The Energy Commodity Chains

The methodology presented in this paper relies on the application of the First Law and the Second Law of Thermodynamics. The following subsections aim to recall the basics of the two laws, to understand their application to the energy chains.

A. The First Law of Thermodynamics

The First Law of Thermodynamics (FLT) expresses the energy balance of a system: hence, it is basically an alternative

[1]Among non-renewable sources we should also enumerate coal and oil and petroleum products. However, since we are analysing the process of the transition towards decarbonisation, they are not taken into consideration.

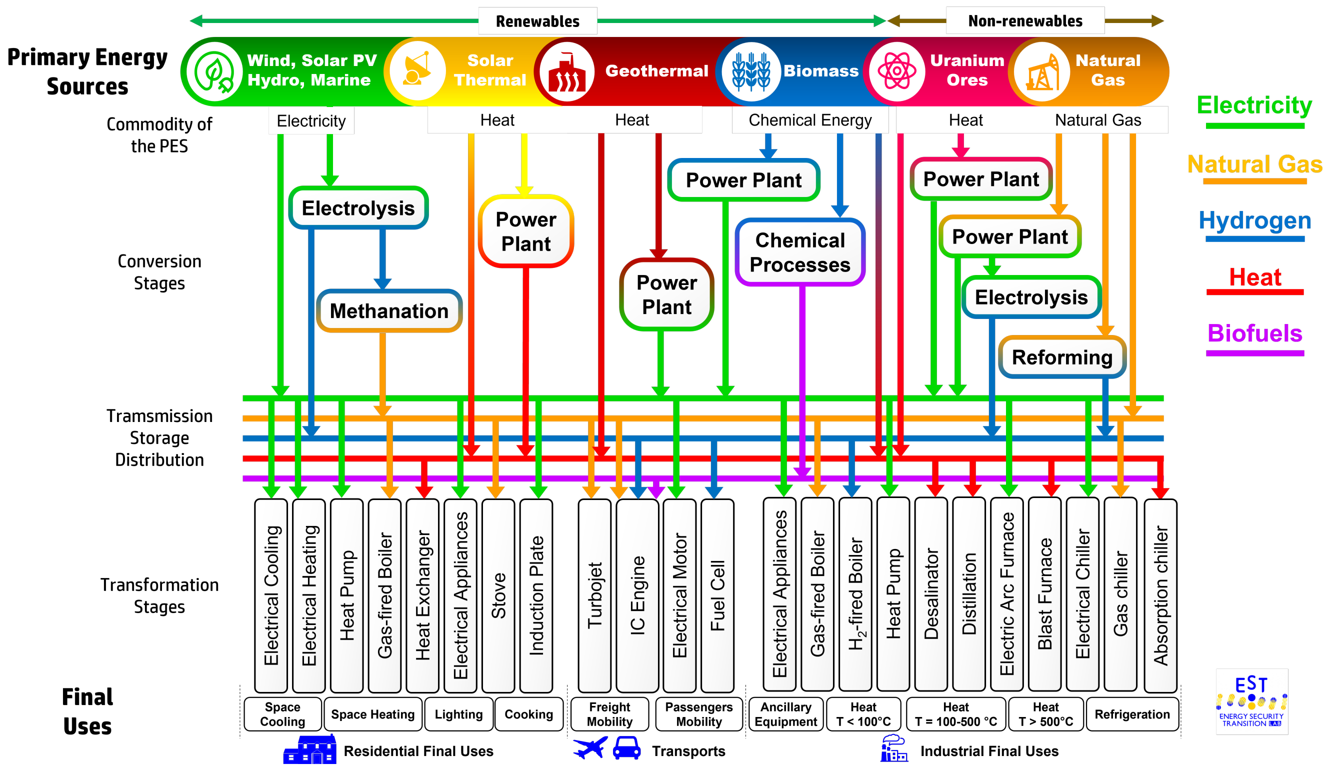

Fig. 1. Multicommodity energy system and energy commodity chains.

formulation of the energy conservation principle [18]. Equation 1 displays the FLT for a generic control volume (CV):

$$\frac{dE}{d\tau} = \sum_{j=0}^{n} \dot{Q}_j + \dot{W}_{el} + \dot{W}_{ch} - \dot{W} + \sum_{i} [\dot{m} \cdot h^0] - \sum_{e} [\dot{m} \cdot h^0] \quad (1)$$

where:

- $dE/d\tau$ is the variation of the *total energy* within the CV.
- $\dot{Q}_j$ is the *thermal flux* exchanged across the boundaries of the CV with the j^{th} thermostat.
- $\dot{W}_{el}$ is the *net electric power* entering the CV.
- $\dot{W}_{ch}$ is the *net chemical power* entering the CV.
- $\dot{W}$ is the *net mechanical power* (also known as *shaft work*) exchanged at the boundaries of the control volume.
- $\dot{m}$ is the mass-flow rate flowing across the boundaries of the CV, where subscripts i and e stand for incoming and exiting fluxes, respectively.
- $h^0 = h + gz + w^2/2$ is called *specific methalpy* (per unit mass), and is the sum of the contributions of specific enthalpy h, potential energy gz, and kinetic energy $w^2/2$, where w is the velocity of the mass-flow rate.

First law (or energy) efficiency is defined as the ratio of energy exploitable in a process (or from a device), to the amount of energy supplied to the same process:

$$\eta_I = \frac{En_u}{En_s} \quad (2)$$

B. The Second Law of Thermodynamics

The Second Law of Thermodynamics (SLT) introduces the concepts of *entropy* and *irreversibility*. The analytical expression of the SLT, which in the beginning existed only in the form of asserts, is an *entropy balance*, as represented in 3 (once again we report the expression for a generic CV):

$$\dot{S}_G = \frac{dS}{d\tau} - \sum_{j=0}^{n} \frac{\dot{Q}_j}{T_j} - \sum_{i=1}^{I} (\dot{m} \cdot s)_i + \sum_{k=1}^{U} (\dot{m} \cdot s)_k \quad (3)$$

where:

- $\dot{S}_G$ is called *entropy generation* and accounts for the presence of irreversibilities within the CV.
- $dS/d\tau$ is the variation of *entropy* within the CV.
- T_j is the *temperature* of the j^{th} thermostat.
- s is the *specific entropy* (per unit mass).

The SLT also sets the boundary between reversible and irreversible processes. Irreversibilities can be external or internal: the first ones basically consist in heat transfers across finite temperature differences between the CV and its surroundings. Internal irreversibilities, instead, include all those phenomena happening within the CV, such as friction, hysteresis, spontaneous chemical reactions, fluid mixing, inelastic deformation, and so on [18]. Only in a reversible process, entropy is conserved.

C. About Exergy and SLT

Irreversibilities reduce the maximum amount of work exploitable from a process and are quantified by the aforementioned *entropy generation*. Reversible processes represent the benchmark at which every actual process should aim, because in a reversible process no work is lost through dissipative phenomena, thus they allow to exploit the maximum amount of work. In thermodynamics, the maximum theoretical amount of work obtainable from a reversible process is also called *exergy* [19]. Exergy is a smart way of merging the first and second laws of thermodynamics. In fact, starting from the assert that mechanical work is the most valuable form of energy, in an exergy balance every other form is converted into its equivalent amount of mechanical work that could be extracted from them. For this reason, exergy is also known as available work. Irreversibilities are instead translated into the concept of lost available work. This means that if energy is conserved, exergy is not. Another crucial aspect to be considered when dealing with exergy is the *definition* of a *reference environment* [20]: in principle, the potential of producing useful work exists between any couple of systems whose conditions are reciprocally different. In exergy analysis, one system is the object of study, whereas the second one is a reference environment, whose pressure, temperature, and chemical composition are chosen and fixed. Hence, when working with exergy, the thermochemical properties of the reference environment must be always properly stated in advance. Exergy efficiency is the ratio of the amount of exergy exploitable in a process when a given quantity of exergy.

$$\eta_{II} = \frac{Ex_u}{Ex_s} \tag{4}$$

It differs from the concept of energy efficiency introduced in Sec. III-A: if *energy efficiency* basically relates to the *quantity of available energy*, *exergy efficiency* is more related to the *quality of the energy fluxes*. This means that the higher the exergy efficiency of a process, the higher the potential work that the downstream fluxes can produce. Carrying out an exergy analysis can help designers in gaining useful insights that a first law analysis alone cannot provide. For example, it can be applied to components whose definition of energy efficiency would be meaningless, such as heat exchangers [20].

More importantly, the possibility of quantifying lost available work for every component of an energy system allows to determine what the most exergy-destroying ones are, therefore where to intervene to reduce irreversibilities as much as possible.

IV. Technologies and Results

Table I displays the conversion, storage, transmission and distribution technologies and infrastructures considered in this study, while in Table II we listed all the devices devoted to supplying energy to the final uses (the coefficient of performance was taken into account for the heat pump). Regarding hydrogen, we considered storage in gasified form and assumed the same transmission and distribution losses of natural gas ducts.

Specifically for the exergy analysis part, we considered also:

- A room temperature $T_r = 293K$ and a temperature $T_e = 273K$ for the external environment. The exergy efficiency of final transformation devices in the space heating sector can be computed as follows:

$$\eta_{II} = \eta_I \cdot \left(1 - \frac{T_e}{T_r}\right) \tag{5}$$

- For sake of simplicity, the calorific values of hydrocarbons were used in place of their chemical exergy, since that the difference between the two values can be considered negligible [19].

Following the simplifying assumptions made for the exergy analysis part, the analytical expression of the Second Law efficiencies of chain steps and transformation devices in which no heat transfer is involved are the same as First Law ones. Fig. 2 displays an example of two energy commodity chains, and Fig. 3 shows a sample of two exergy commodity chains. The complete computational results are then illustrated in Sections IV-A and IV-B.

TABLE I
SYNOPTIC VIEW OF THE CONSIDERED TECHNOLOGIES AND DEVICES AND THEIR RELATIVE EFFICIENCIES

Chain Step	Technology	Commodity	η_I	η_{II}
Conversion	Alkaline Electrolyser	Hydrogen	0.60 [21]	0.60
Storage	Li-ion Battery	Electricity	0.94 [22]	0.94
Storage	Pressure Vessel	Hydrogen	0.85 [23]	0.85
Transmission	Power Line	Electricity	0.98 [24]	0.98
Transmission	Gas Duct	Natural Gas	0.95 [25]	0.95
Distribution	Power Line	Electricity	0.93 [26]	0.93
Distribution	Gas Duct	Natural Gas	0.99 [27]	0.99

TABLE II
CHARACTERIZATION OF FINAL TRANSFORMATION DEVICES

Device	Final Use	Commodity	η_I	η_{II}
Heat Pump	SH[a]	Electricity	3 [28]	0.20
Condensing Boiler	SH	Natural Gas	0.90 [29]	0.06
Electric Heater	SH	Electricity	0.95 [30]	0.06
Condensing Boiler	SH	Hydrogen	0.90 [31]	0.06
Electric Motor	PT[b]	Electricity	0.85 [32]	0.85
ICE[c]	PT	Natural Gas	0.40 [33]	0.40
Alkaline Fuel Cell	PT	Hydrogen	0.55 [34]	0.55
ICE	PT	Hydrogen	0.37 [35]	0.37

[a]Space Heating [b]Passengers' Transports [c]Internal Combustion Engine

A. Energy Analysis

Table III displays the results, in terms of overall efficiency of the chain, of the energy analysis.

Regarding space heating, heat pumps are the most energy efficient devices among the considered technologies. In fact, gas-fired condensing boilers and electric heaters require a three times larger primary energy supply to feed final uses with an equal amount of energy. Hydrogen-fired boilers instead need almost a six-times higher quantity of energy.

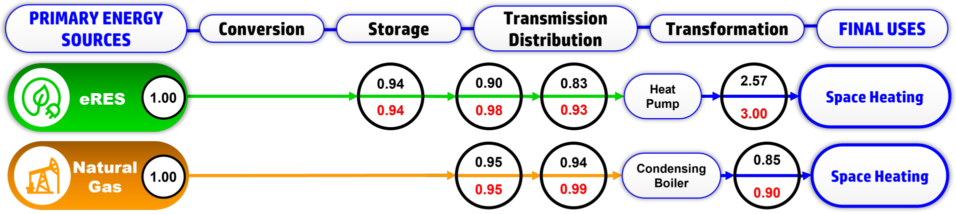

Fig. 2. Example of energy commodity chains.

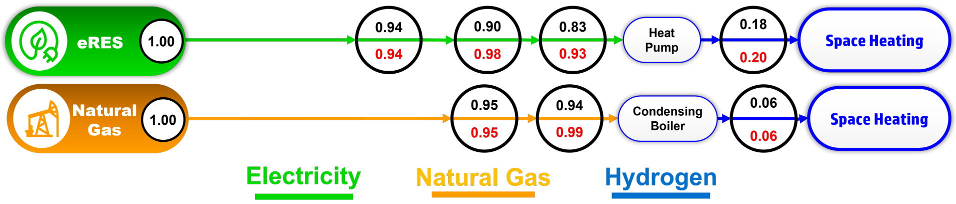

Fig. 3. Example of exergy commodity chains.

TABLE III
COMPUTATIONAL RESULTS OF ENERGY ANALYSIS

Chain ID	***Device***	***Final Use***	***Commodity***	***Chain Efficiency***
1	Heat Pump	SH	Electricity	2.57
2	Condensing Boiler	SH	Natural Gas	0.85
3	Electric Heater	SH	Electricity	0.81
4	Condensing Boiler	SH	Hydrogen	0.43
5	Electric Motor	PT	Electricity	0.73
6	ICE	PT	Natural Gas	0.38
7	Alkaline Fuel Cell	PT	Hydrogen	0.27
8	ICE	PT	Hydrogen	0.18

In the field of light duty transports, the electric motor is the best performing technology, as it needs less than half the amount of energy required by fuel cell vehicles, and around one quarter of the quantity of energy absorbed by a hydrogen-fired ICE. A lower, but still considerable gap exists between electric motors and gas-fired ICEs, as the latter require around twice the amount of primary energy to match the performances of an electric motor.

B. Exergy Analysis

Table IV displays the results, in terms of overall efficiency of the chain, of the exergy analysis.

TABLE IV
COMPUTATIONAL RESULTS OF EXERGY ANALYSIS

Chain ID	***Device***	***Final Use***	***Commodity***	***Chain Efficiency***
1	Heat Pump	SH	Electricity	0.18
2	Condensing Boiler	SH	Natural Gas	0.06
3	Electric Heater	SH	Electricity	0.06
4	Condensing Boiler	SH	Hydrogen	0.03
5	Electric Motor	PT	Electricity	0.73
6	ICE	PT	Natural Gas	0.38
7	Alkaline Fuel Cell	PT	Hydrogen	0.27
8	ICE	PT	Hydrogen	0.18

For space heating, also in this case heat pumps stand out as the most efficient devices among the considered technologies, due to the fact that they do not involve any combustion, which is amongst the most exergy-destroying processes [20]. Generally, the efficiencies of the whole chain in the space heating field are considerably lower than their energy counterparts, due to relatively low Carnot factors. In fact, the potential of the incoming flow of exergy is used to bring the room temperature only $20°C$ far from that of the reference environment. Hence, we may say that the available work potential is underexploited.

It is possible to draw some insightful considerations also for the passengers' transport sector, regardless the fact that the overall chain efficiencies are the same. Electric motors are a preferrable choice, because they convert electricity into shaft work: therefore, the quality of the incoming energy flux is not downgraded to less valuable forms of energy. Considering the whole chain, gas-fired internal combustion engines are the second most performing devices. However, fuel cells have an intrinsically higher exergy efficiency, due to the presence of a combustion reaction in ICEs, regardless the hydrocarbon used as a fuel. At the same time, the fuel cell chain lags behind the gas one because electrolysis is a relatively inefficient process.

V. CONCLUSIONS

This paper focused on the energy efficiency aspect of different energy commodity chains. The computational results suggest that electricity might stand out as a preferrable commodity in the transition cocktail. In fact, it is the only carbon-free primary commodity that can directly be used to supply the final uses and, in terms of exergy, it is as valuable as mechanical work. On the contrary, hydrogen produced via electrolysis lags behind both electricity and natural gas, because electrolysis itself is a significantly inefficient process, both in terms of energy and exergy.

Nevertheless, hydrogen might carve out a crucial role in the energy transition, especially for the possibility to store it for a long time, which may increase the overall energy system security.

The formulation of an exhaustive answer to the problem of the best commodity mix for the energy transition requires a broader analysis, which not only takes into account technical- and efficiency- related aspects, but also analyses the socioeconomic implications, as well as the environmental impacts of the various commodity chains. Moreover, considering the growing importance of the topic of energy security of supply, considerations about the geographical allocation of both the raw materials and the finished products required to build the necessary energy infrastructures and devices will gain more and more value. All the above aspects will be integrated as additional problem dimensions in our future works, with the aim to refine the output ranking related to the different multicommodity energy chains.

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