Energy Storage System Hybridization Algorithm for Mobility Applications Based on Future Battery and Fuel Cell Technologies

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Abstract—**Shifting the mobility paradigm from fossil fuel to electric propulsion system poses several challenges to a large extent attributed to the low energy density of storage systems. However, technology improvements and an accurate combination of new propulsion systems can facilitate the electrification of the mobility sector. For the first time, a hybridization algorithm is developed to evaluate the optimal configuration of future Energy Storage System (ESS) to facilitate the design of systems such as aircrafts or ships. The algorithm is based on operational behaviors and high-level performances to determine the optimal solution through a standard random search of the input variables. To feed the algorithm, forecasts including estimated performances are carried out on new energy storage technologies such as Fuel Cells (FCs), batteries, and hydrogen storage. The hybridization algorithm is then applied to the design of a 50 passengers' regional electric aircraft in 2040. The results suggest that the best ESS includes a Solid-State Battery (SSB) of 457 kWh, a 1788 kW Solid-Oxide Fuel Cell (SOFC) plant and consumes 190.9 kg of hydrogen. This configuration appears to be the optimal trade-off to minimize weight, volume, and costs.**

Keywords— Hybridization, energy storage system, battery, fuel cell, mobility, aviation, optimization, sizing, forecasts.

I. Introduction

The Intergovernmental Panel on Climate Change (IPCC) has outlined the need for drastic reductions in Greenhouse Gases (GHG) emissions of 63% by 2050 to limit global warming below 2°C [1]. Emissions reductions achieved across all sectors are critical and particularly in the mobility sector, which is the main contributor to GHG emissions. The key to reduce emissions in transportation relies in drastically accelerating the transition from fossil fuel-based systems towards electrified alternatives. However, this electrification is hindered mostly by the limited energy and power density of the energy storage technologies. Hybridization, or the combination of multiple energy storage technologies, has the potential to improve performances, reliability, robustness, and sustainability of the overall system. Despite the increase of complexity, the development of hybrid electric propulsion has been receiving increased attention with various vehicles such as FC-battery powered aircrafts or battery-combustion engine in vehicles [2]. These new interfaces infer different design and novel optimization methods to identify impactful variables, constraints, and objectives. Different articles have already presented hybridization algorithms based on existing technologies for mobility applications to optimize quantitative measures such as weight or costs [3], [4]. To our knowledge, hybridization algorithms focusing on future ESS have yet to be assessed. Such model would be extremely relevant for applications which require long term technical assessments such as aircrafts or ships.

The first step consists of technological forecasting. Based on theoretical limits of current technologies, development rates in previous years, promising new materials under study and extrapolation techniques, key performance parameters such as energy and power density are evaluated over three-time horizons. Forecasts for batteries, FCs and hydrogen storage technologies are provided with their performances and behaviors to be later integrated into the hybridization algorithm. Then, the algorithm's structure will be described to reveal its functioning, versatility, and interdependences between sub-systems. Finally, the algorithm will be applied to design a hybridized ESS for an electric regional aircraft of 50 passengers projected for 2040.

II. Energy Storage Technologies

Multiple energy storage technologies are defined along with potential innovations and useful performance indicators for three future timelines (2030/2040/2050+). The forecasts aim to bring a perspective on the evolution of energy storage technologies to be integrated in the hybridization algorithm to design a potential ESS. However, the presented technologies are still in early stages of developments and the future of the field may differ from these predictions.

A. Battery technology

Batteries are widely considered as one of the most valuable components for a complete decarbonization of the society. A battery is a device that stores chemical energy and converts it into electrical energy. It consists of a cathode (positive electrode), an anode (negative electrode), a separator, and the electrolyte. Different electrodes are available but, forecasts suggest that lithium (Li) should remain one of the main components to fulfil high-energy and high-power applications [5]. The scientific community reached this

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consensus because Li is the 3rd lightest element (lightest metal) while having the lowest reduction potential allowing Li cells to reach high potentials and high gravimetric energy densities [6].

In 2030, Li-ion batteries are expected to remain the main technology. The cathode should be composed of a lithium alloy which is $N_8M_1C_1$ (80%Nickel, 10% Manganese and 10% Cobalt). Further improvements on the cathode such as specific coatings or doping strategies are under developments which will improve lifetime, safety, and performances of the cell [5]. The anode will remain graphite with a small percentage of Silicon (~10%) which is the current state of the art. Silicon provides better energy density for the cell, but also brings other challenges such as volumetric expansion and lower lifetime.

By 2040, Solid-State batteries (SSBs) and Lithium Sulphur (Li-S) batteries will likely become a standard solution as they are currently being under significant research and pilot lines are already projected. SSBs have a similar composition as Li-ion, but the liquid electrolyte is substituted with a solid one. For high performance, Sulphide-based inorganic crystalline electrolytes are the most likely solutions to succeed thanks to the high conductivity at relatively low operating temperature (60-80 °C)[7]. The main drawbacks reside in the high reactivity with electrodes and its toxicity. Interestingly, on-going developments on cathode and anode active materials from Li-ion are expected to be largely transferrable to SSBs. Therefore, Li-rich oxides cathodes should remain the mainstream solution in the future. The final choice of the specific cathode chemistry would depend on the application's requirements. Mobility applications typically require high specific power and high energy density. These demands could be fulfilled by cathode materials composed of lithium-manganese-nickel oxides (LMNO) or $N_8M_1C_1$. On the anode side, developments are expected to occur in two different phases. First, the anode should remain graphite with silicon particles as the major challenge relies in developing a solid electrolyte with sufficient conductivity. Second, solid electrolyte should enable the implementation of Li metal anodes which would drastically improve the energy density of the battery cell (specific capacity of 370 mAh/kg vs 3850 mAh/kg for a Carbon and a Lithium metal anode respectively) [8].

Li-S batteries have received lately an increased attention thanks to their extremely high theoretical energy density (~2700 Wh/kg) which is 5 times higher than the theoretical limit of Li-ion batteries [9]. While this value is significantly lower in practice, the technology has already demonstrated great performances in a technologically relevant cell format (e.g., 470 Wh/kg) [10]. This range of performances is extremely important to enable new applications such as aviation and maritime. In addition, Sulphur is an abundant, cost effective and environmentally friendly material which is very beneficial to reduce the environmental impact of batteries and thus, of the mobility sector [11]. In contrast to SSBs and Li-ion batteries which employ an intercalation mechanism, Li-S cells operate by a conversion mechanism. Elemental Sulphur (S) (cathode) and Li (anode) react to form polysulfides as shown in (1).

$$S_8 + 16e^- + 16Li \leftrightarrow 8Li_2S \qquad (1)$$

Due to the complex working principle, many challenges need to be overcome such as polysulfide shuttle effect which causes a loss of active S from the cathode, low solubility of polysulfides which impact the discharge current or significant volume expansion which influences drastically the lifetime of the cell [12]. The potential of cost reduction brought by the implementation of S most likely will accelerate the commercialization and widespread use of Li-S batteries. Forecasts suggest that with comparable performances, the cost of a Li-S cell could become just half of a Li-ion cell, as cathode materials are the main reason for the high cost of LIBs (i.e., Nickel, Cobalt, Aluminium…) [9].

From 2050, Li-air batteries and particularly non-aqueous Li-air chemistries feature great potential for electric mobility. The basic principle is that the anode (lithium metal) reacts with the cathode, which consists of oxygen, to produce lithium peroxide. During the charging process, the lithium peroxide is broken up in lithium and oxygen which allows the cell to be re-used. The reaction is detailed in (2) below.

$$2LiO_2 \leftrightarrow Li_2O_2 + O_2 \qquad (2)$$

Li-air cells show extremely high energy density, theoretically, up to 3460 Wh/kg. However, in practice, G. Girishkumar, B. McCloskey, A. C. Luntz, S. Swanson and W.Wilcke predicted that Li-air could only reach up to 1700 Wh/kg due to the weight penalty of packaging and structural components [13], [14]. Li-air batteries are still facing plenty of challenges such as low electrical efficiency, low discharge C-rates and low lifetime. Although no practical applications exist yet, Li-air batteries were already considered as a candidate to power the VoltAir aircraft planned designed by EADS [13]. In this paper, it is expected that this technology will take a significant time to reach maturity due to its complexity, and therefore, will only become relevant by 2050 [15].

In TABLE I. , battery cell forecasted performances can be seen for three timelines. Additionally, power densities are calculated considering a nominal C-rate of 2, 4, 1.5 and 2 for Li-ion, SSB, Li-S and Li-air respectively.

B. Fuel Cell technology

Although FC based systems represent a large potential for meeting the challenges of an environmentally sustainable energy supply for mobility applications, actual implementations remain limited. The majority of FC systems rely on generating power through hydrogen, which has long been hailed as the future fuel thanks to its high gravimetric energy density (almost three times that of kerosene) [16]. Large investments (e.g., in Japan or Europe) and advances in materials science improving efficiencies and power densities are making FCs a viable option for mobility applications such as ships or aircrafts [17]. However, even though laboratory performances have been quite promising, the transfer of knowledge from laboratory to industrial scales is challenging due to low manufacturing volumes and high costs of FCs. This article focuses on technologies such as Proton Exchange Membrane Fuel Cell (PEMFC) and Solid Oxide Fuel cell (SOFC) because they feature the best performances related to power density and efficiency and attract the most interests by the scientifical community.

TABLE I. BATTERY PERFORMANCES FORECASTS

		2030	2040		2050	
		Li-ion	*SSB*	*Li-S*	*SSB*	*Li-Air*
Energy density	*Gravimetric [Wh/kg]*	370	650	750	650	1050
	Volumetric [Wh/L]	700	1105	1050	1105	1785
Power density	*Gravimetric [Wh/kg]*	740	2600	1125	2600	2100
	Volumetric [Wh/L]	1400	4420	1450	4420	3570

PEMFC or more precisely low temperature PEMFCs (LT-PEMFCs), are the most commercialized technology due to its low operating temperature, short start time, and ease of use of its oxidant (i.e., atmospheric air). PEMFCs are already used in many systems, such as the first usable hydrogen-electric hybrid car in 2014 or more recently in the NEXP car from Hyundai, which has an autonomy range of 570 km [18]. A single FC consists of a so-called bipolar plate with an anode and a cathode side, two gas diffusion layers (GDLs) a catalyst-coated membrane between the GDLs. Normally, the catalyst coated membrane and the gas diffusion layer form the membrane electrode assembly.

SOFCs are also gaining attention thanks to their high electrical efficiency (above 60%) and the possibility to use alternative fuels (i.e., CH_4, $NH_{3...}$). SOFCs are already used in specific applications such as power backups for hospitals or data centers, but only few prototypes dedicated to mobile applications have been made. SOFCs employ a non-porous "solid ceramic" electrolyte such as zirconium oxide stabilized with yttrium oxide and operate at high temperatures (600-1000 °C) [19]. The oxygen/air is fed to the positive electrode (cathode), and the mobility of the ions is initiated by the non-porous solid electrolyte. In this paper, SOFCs will only be considered with pure hydrogen due to the need for high energy densities in mobility applications.

Multiple technological gaps must be addressed to allow FCs to reach mass market utilization. Both technologies will require a significant weight reduction of the balance of plant (BoP) to be successful as auxiliaries are currently complex and heavy. Other developments are focusing on increasing the voltage or the maximum surface power density. SOFCs must be specifically designed to reduce thermal stress build-up in the thin layer electrode and electrolyte as cracking interfacial delamination occur during the preheating phase. Additionally, the high temperature implies the use of high thermal resistant materials such as nickel, Yttria-stabilized zirconia and metallic cathode which often features high gravimetric densities.

The evolution of the gravimetric and volumetric power densities at the stack level can be seen in TABLE II. For FCs, voltage and efficiency curves are also important to define the stack working point and the corresponding power and hydrogen consumption of the system.

C. Hydrogen storage

Hydrogen receives a lot of attention because it has the highest energy per mass amongst standard fuels (33.33 kWh/kg), but issues remain regarding its reactivity with ambient air, the difficulty of storage and its low volumetric density as a gas. For sake of simplicity and relevance regarding mobility applications, only gaseous and liquid storage will be assessed in this article.

TABLE II. FUEL CELL PERFORMANCES FORECASTS

Stack power density	Technology	2030	2040	2050
Gravimetric [kW/kg]	*SOFC*	0.5	1.5	2.5
	PEMFC	2.5	4.4	6.2
Volumetric [kW/kg]	*SOFC*	1	2	3
	PEMFC	3.1	4.5	5.3

1) Gaseous Storage

The first and most developed solution consists of commonly storing hydrogen in a gaseous state in pressure vessels between 200 and 700 bar to achieve sufficient density. With these pressure conditions, the hydrogen density is still rather small at ambient temperature (below 40 g/L) but remains far lighter than the container's weight designed to withhold the resulted stress. Nowadays, only type IV vessels composed of a polymer liner fully overwrapped with composite material are commercialized. The polymer liner is thin and constitutes the hydrogen-tight barrier. For the future of hydrogen vessels, a next design of pressure tank would be a liner-less composite tank with an expected 10-20% decrease on weight. The main challenges are dedicated to guarantee a low permeation rate through the thermoset matrix of the composite and to wind the composite without the liner acting as a mandrel. The technology is not mature yet but is under development in several companies [20].

2) Liquid Storage

Storage of hydrogen in its liquid form requires cryogenic temperatures since the boiling point of hydrogen at 1 atm is −252.8 °C. In these conditions of temperature and pressure, liquid hydrogen has a high density of 70.8 kg/m^3 in comparison with the density of 40.2kg/m^3 at 700 bar and 15°C. The main issues of this storage strategy are linked to the high consumption of energy and complex equipment needed to liquify hydrogen. Although cryogenic hydrogen tanks are already used regularly in aerospace launchers, there is a lack of knowledge regarding the fatigue behaviour as the tanks are designed for a single usage. Regarding mobility applications, the tank will require to be filled many times, so the mechanical and thermal fatigue behaviour will become a major criterion to consider.

Due to the differences in technological readiness levels, gaseous storage is considered for 2030 and 2040, whereas liquid storage will only be implemented for systems starting from 2050. E. Rivard, M. Trudeau and K. Zaghib reviewed the current standard for different hydrogen storage technologies and stated that gravimetric index of 5.7% and 7.5% were reached for gaseous and liquid storage respectively [16]. Therefore, according to these values and the information presented above, the forecasted gravimetric indexes are shown for both technologies in TABLE III.

D. Costs forecasts

The cost of a technology is a major criterion in achieving wide market utilization. Therefore, forecasts on cost have been carried out for each technology mentioned in chapter II and the values for each timeline can be seen in 0

TABLE III. HYDROGEN STORAGE PERFORMANCES FORECASTS

	Technology	2030	2040	2050
Gravimetric Index [%]	*Gaseous*	8	15	16
	Liquid	15	30	42

TABLE IV. COSTS FORECASTS [16], [21], [22]

Technology	Unit	2030	2040	2050
Li-ion	$/kWh	100	85	72
SSB		115	83	70
Li-S		110	79	60
Li-air		104	74	61
SOFC	$/kW	n/a	1525	830
PEMFC			1050	750
Gaseous storage	$/$kg_{H2}$	n/a	1090	633
Liquid storage		n/a	390	150
H_2	$/kWh	0.14	0.08	0.05

III. HYBRIDIZATION ALGORITHM

The hybridization algorithm's goal is to derive the optimal sized FC-battery system to fulfill the desired application power profile. The difference with previous optimization algorithms resides in the use of projected performances of technologies. This nuance implies that the user might not be able to base its analysis on a complete set of measured characteristics, but only on high level values of the system (e.g., system power density). The resulting ESS can become a useful element for deeper assessments of systems such as future hybrid electric aircrafts or cargo-ships. The algorithm's structure is composed of three distinct sections (Fig. 1): input processing (in yellow), simulation engine (in blue) and Key Performances Indicators (KPIs) calculations (in purple).

The first section regroups all inputs data required to run the hybridization algorithm. A standard power profile required by the application shall be provided along with a potential set of constraints on the ESS (e.g. maximum weight…). Then, a database of technologies was gathered focusing on the evolution of batteries, fuel cells and hydrogen storage for 3 horizons – 2030, 2040, 2050+. Each technology is defined as its own class with performances, behavior and constraint indications corresponding to the defined variables as in TABLE V. An appropriate selection of the technologies is also necessary, and the list of the available classes is shown in Fig. 2.

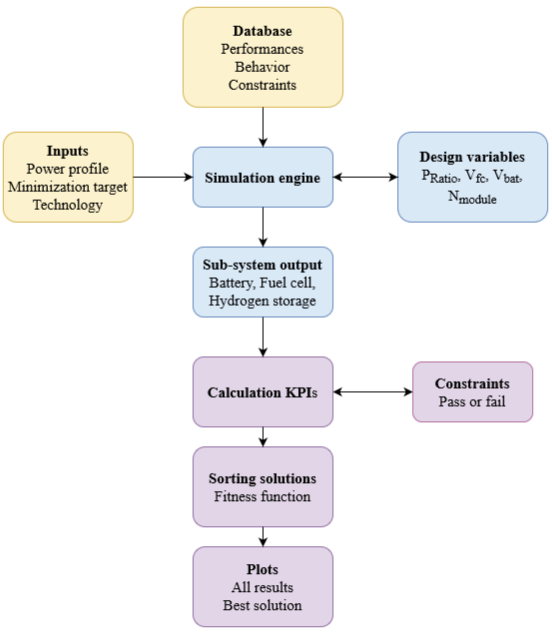

Fig. 1. Hybridization algorithm's structure.

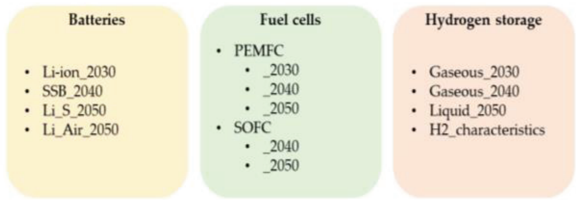

Fig. 2. List of energy storage technologies available.

TABLE V. CLASS STRUCTURE

Class		
Battery	***Fuel Cell***	***Hydrogen storage***
Voltage curve – B	OCV curve - B	Fuel LHV/HHV – P
Energy density – P	Electrical efficiency - P	Gravimetric index – P
Maximum C-rate - C	Cell area – B	Volumetric index – P
Efficiency – P	Maximum surface current - C	Tank diameter - B
	Fuel utilization – P	
	Stack PD – P	
Costs: Acquisition Operation Maintenance	Costs: Acquisition Operation Maintenance	Costs: Acquisition Operation Maintenance
B: Behaviour, C: Constraint, P: Performances		

The second section (in blue in Fig. 1) refers to the simulation engine which creates a hypothetical ESS through a random search of variables. Random search is an approach to optimization where random combinations of variables (within defined ranges) are applied to design and influence KPIs of the ESS (e.g., weight or efficiency). This simple method can be used in combination of any optimization method to find the global minima and does not require any prior knowledge about the relationship between the variables. The main drawback of a random search is its inefficiency, but, thanks to the low number of variables, the computing speed is considered sufficient for this application. The decision variables are the splitting ratio of maximum power (P_{ratio}) defined as P_{fc_max}/P_{max} , the voltage of the battery and FC system (V_{bat}, V_{fc}) and the number of modules (n_{module}). The simulation engine starts by generating a new set of decision variables. The input power profile and P_{ratio} are then processed to create distinct power profiles for the battery and FC system such that the latter is used at a maximum of 80% of its rated maximum power, except when the power demand cannot be fulfilled otherwise. This method was selected in order to optimize the FC efficiency as higher losses and higher degradation arise when they operates close to full power. With a similar intention, a safety factor of 20% is added to the battery pack to guarantee that the system is oversized at the beginning of life. This safety factor aims to minimize the battery degradation and to account for unforeseen events. The FC and battery systems are then designed based on the performances indicated by the technology class selected. Technology performances were provided at the unit level (battery cell and FC stack), and do not reflect the system performances. Therefore, a unit to system coefficient (ε_{sys}) has been included to up-scale to system values and the evolution of this coefficient can be seen in TABLE VI.

TABLE VI. UNIT TO SYSTEM COEFFICIENTS

Unit to system - ε_{sys}		2030	2040	2050
Battery	***Gravimetric***	80%	90%	90%
	Volumetric	60%	70%	75%
SOFC	***Gravimetric***	40%	75%	75%
	Volumetric	50%	50%	50%
PEMFC	***Gravimetric***	30%	32%	35%
	Volumetric	18%	20%	30%

For both sub-system, the number of cells required in series and parallel is calculated and a weight penalty is integrated for each additional module due to the need for additional components (e.g., cables). Operational data such as airflow, fuel consumption, water emissions or heat generation are estimated using the voltage and efficiency curves of the FC. With these operational data, the fuel tanks can be designed to store the required amount of hydrogen. Finally, the cost of each sub-system is also computed considering acquisition, installation, operation, and maintenance. Degradation has yet to be implemented.

The third section of the algorithm focuses on calculating KPIs, computing the fitness function and plotting all relevant results. System KPIs are calculated for all solutions such as costs, weights or volumes. The optimal ESS solution is then selected based on a fitness function that combines a weighted formulation and is described in (3).

The following chapter presents the algorithm's results obtained for the design of the ESS for an electric regional aircraft in 2040.

IV. DESIGN OF THE ESS FOR AN ELECTRIC AIRCRAFT IN 2040

The energy storage technologies selected for the design of an electric regional aircraft in 2040 are SSBs, SOFCs and gaseous storage of pure hydrogen. The power profile is composed of 9 flight phases with their own durations and power requirements, namely: take-off, climb, cruise, descent, second climb, alternate, second descent, loiter and landing [23]. The initial power profile can be seen in Fig. 4 with the purple curve.

After having generated all the solutions by randomly varying the decision variable in the appropriate ranges, the solutions are evaluated according to the objective function defined in (3).

$$f_{objectiv} = 0.55 * \frac{m_{sol}}{\min(\mathrm{m_{all}})} + 0.15 * \frac{V_{sol}}{\min(\mathrm{V_{all}})} + 0.3 * \frac{C_{sol}}{\min(\mathrm{C_{all}})} \quad (3)$$

With m_{sol} , V_{sol} and C_{sol} being the weight, volume and costs of a solution, whereas m_{all} , V_{all} and C_{all} represent a list including the results of all generated solution for the weight, volume and cost respectively.

The best ESS configuration is isolated with a green dot in Fig. 3 and represents a solution where 30% of the maximum power is provided by the battery. Smaller batteries seem to be preffered because of the heavy weight carried out by SSBs. The best ESS (according to the fitness function) is composed of a 457 kWh battery, a 1787.5 kW SOFC plant and consumes a total of 190.9 kg of hydrogen. The battery pack is composed of 4 modules with 2 connected in series and 2 in parallel (2S2P). Each module includes 666 cells with a 37S18P configuration. Additionnaly, the FC plant is composed of 9 stacks connected in series, where each stack includes 94 cells in series. The overall weight of the ESS is 3534 kg for a volume of 4805 liters.

Fig. 4 depicts the power splitting between both sub-systems. The battery supports greatly the FC in high power phases like take-off or climb, but only provide a minor contribution in long and high energy phases. This phenomenon can be greatly attributed to the extremely high energy density of hydrogen compared to batteries (33.33kWh/kg vs 0.65kWh/kg).

Fig. 5 shows the composition of each sub-system as a function of the weight and volume. Batteries and FCs account for the majority of the weight, but, hydrogen and fuel tanks occupies larger volumes. An interesting result is also that the weight of the hydrogen appears to contribute only slightly to the overall weight of the ESS.

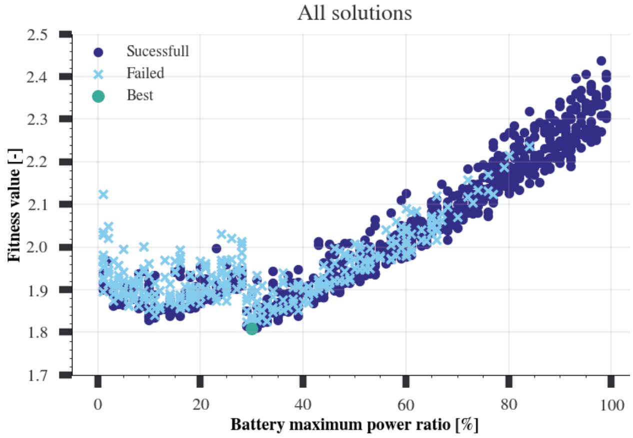

Fig. 3. Scatter plot showing the fitness value for all simulated ESS as a function of the battery maxium power ratio.

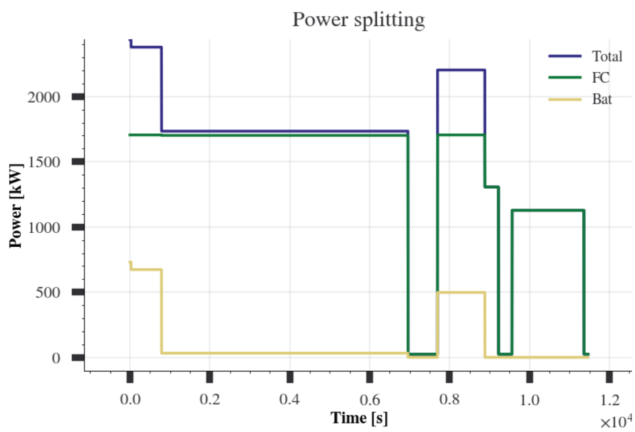

Fig. 4. ESS power profiles representing the best solution for an electric regional aircrafts in 2040.

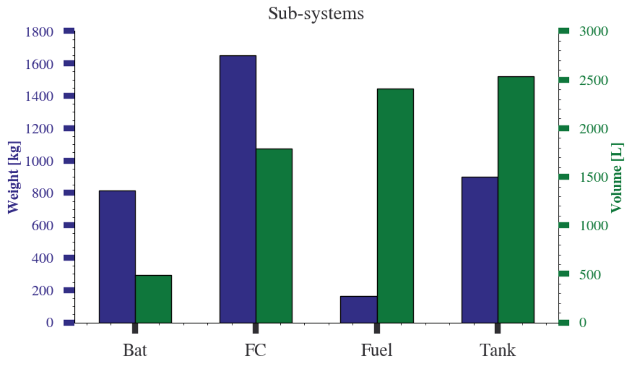

Fig. 5. Weights and volumes of the different sub-systems for the best ESS solution.

V. Conclusion

The evolution of three major energy storage technologies have been assessed to provide forecasts on their performances and costs. Improvements of the mentioned technologies are anticipated to be significant in the future to fulfill the ambitious goal of a decarbonized society. The outcomes of the forecasts were feed in a novel hybridization algorithm to design future ESS based on a random search of decision variables. The algorithm was also detailed to explain its functioning and structure. The best ESS according to a specific fitness function was computed for a regional electric aircraft of 50 passengers in 2040. The results highlighted the impact of each sub-system on KPIs such as weight, volume and cost. The best ESS was found to be composed of a 457 kWh SSB, a 1787.5 kW SOFC plant and consumes a total of 190.9 kg of hydrogen.

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