

Configuration Optimization of a Hydrogen-Kerosene Hybrid Combustion Aircraft Retrofit

Caleb Akhtar Martinez* and Jerome P. Jarrett†

University of Cambridge, Cambridge, CB2 1PZ, England, United Kingdom

With the deadline to reach net-zero quickly approaching, the aviation industry will soon have to shift away from kerosene aircraft. One of the candidate zero-emissions technologies for future aircraft is hydrogen. However, due to the technology being yet immature, the implementation of hydrogen on aircraft is expected to be a long-term endeavour. To accelerate this process, a study has been conducted to evaluate the feasibility of hydrogen-kerosene hybrid combustion as a stepping stone towards full hydrogen implementation. Three goals have been defined: to estimate first-order performance of future hydrogen combustion aircraft, to bring understanding to the hydrogen combustion design space, and to identify a potential pathway for the implementation of hydrogen combustion. To achieve these, simulations have been run using a computational model of a hydrogen retrofit of a ATR 72-500 with engines capable of hybrid combustion. An optimization approach was used to explore this new design space without biases. To accurately reflect the importance of each optimization objective, Tabu Search with Multiple Dominance Relations was chosen as the optimizer. The results of this investigation have revealed fundamental trade-offs in the retrofit design space and provided a set of optimized aircraft of varying hybridisation fraction that can pave the pathway towards full hydrogen implementation in aircraft.

I. Nomenclature

$\leq_k$	=	k -th Binary relation
β	=	Average climb angle
η_{prop}	=	Propulsive efficiency
η_{th}	=	Turbo-engine thermal efficiency
η_{ov}	=	Product of the turbo-engine thermal efficiency and propulsive efficiency
η_{req}	=	Storage efficiency of a liquid hydrogen tank
θ_d	=	Glide angle
λ	=	Cylinder length to total length ratio of a hydrogen tank
ρ	=	Density
Φ_{H_2}	=	Proportion of power from hydrogen (hybridisation fraction)
ϕ	=	Ratio of the major and minor axis lengths of an ellipse
ψ	=	Spheroid geometry parameter
a	=	Hydrogen tank axial cross-section major radius
$BSFC$	=	Brake-Specific Fuel Consumption
b	=	Hydrogen tank spheroid axial radius
C	=	Specific energy
c	=	Hydrogen tank cross-section minor radius
D	=	Drag force
E	=	Work done
f	=	Cruise power to descent power proportionality factor
g	=	Acceleration due to gravity
h	=	Cruise altitude
JAI	=	Kerosene

*Ph.D. Candidate, Department of Engineering, ca525@cam.ac.uk

†University Senior Lecturer, Department of Engineering, Senior Member AIAA.

KE	=	Kinetic energy
L	=	Lift force
L/D	=	Lift-to-drag ratio
LH_2	=	Liquid hydrogen
l	=	Length
$\dot{m}$	=	Mass flow rate
M	=	Cruise Mach number
n_{pax}	=	Number of passengers
n_{seats}	=	Number of seats
P	=	Power
P_{max}	=	Maximum single engine power
PE	=	Gravitational potential energy
$PF(\mathbb{X})$	=	Pareto front
$\mathbb{Q}$	=	Performance space
$\hat{R}_k(x)$	=	k-th Rank
r_{max}	=	Maximum allowed hydrogen tank radius
s	=	Aircraft range
T	=	Time
V	=	Volume
V_2	=	Minimum flight speed
W	=	Mass
W_{CO_2}	=	In-flight carbon dioxide emissions
w	=	Distance travelled in intrinsic coordinates
$\mathbb{X}$	=	Design space
x	=	Design vector

II. Introduction

AVIATION has arguably been one of the most critical sectors in facilitating the global society we currently live in and, although currently responsible for about 2.5% of all anthropogenic CO_2 emissions, the rising demand for air travel has resulted in an exponential increase in its net CO_2 emissions over the past eighty years [1]. If these trends continue, aviation has the potential of becoming one of the leading polluters globally. For this reason, the UK is aiming to de-carbonise the aviation industry by 2050 [2]. However, unlike most other industries, the path to decarbonisation in aviation is rather ambiguous; there are many candidate technologies yet there is no industry-wide consensus as to which of them could be an effective replacement for kerosene.

Sustainable Aviation Fuels (SAFs) are one of the candidate technologies considered to replace kerosene. With current Rolls-Royce Trent engines certified to operate with a 50:50 blend of SAFs and kerosene [3], and a number of production methods already being certified [4], SAFs have the potential to reduce aviation emissions in the shortest time possible. However, projections indicate that the UK could meet 32% of its demand for kerosene with domestically produced SAFs [5]. Limited by production, SAFs are not likely to be the single solution to the decarbonisation of aviation. Alternative technologies must therefore be considered to decarbonise the remaining share of the sector.

Current battery energy densities are approximately 2% of that for kerosene [6]. Although electric vertical take-off and landing prototype aircraft are already flying [7], they are to serve an emerging market, as opposed to the existing market. Drastic improvements will have to be made if battery-electric aircraft are to fly current commercial routes. For this reason, battery-electric aircraft have not been considered in this study.

Hydrogen has a specific energy 2.5 times that of kerosene, but roughly occupies 4 times the space of kerosene [8]. Despite this, the CRYOPLANE project concluded that hydrogen is a feasible technology for aviation [9]. However, as in other efforts, only bespoke hydrogen aircraft designs were considered [9–11]. This suggests that hydrogen is a promising candidate solution to account for the market share not accounted for by SAFs, once the technology matures.

Reaching maturity in hydrogen aircraft technologies is a two-step process: both the hydrogen technologies and the bespoke aircraft configurations must be developed and certified. In order to simplify the problem, several efforts have focused on making hydrogen aircraft with the traditional tube-and-wings configuration [11, 12]. Solving the hydrogen problem for short ranges, where volume is more constrained and iterations are cheaper, will provide the industry with the key unlocks required to implement hydrogen at larger scales. This agrees with the incremental strategy chosen by

ZeroAvia for retrofitting existing aircraft with hydrogen [13]. Similarly, hydrogen research in academia is being done for the 60-80 passenger range for regional turboprop aircraft, taking the ATR 72 as a reference design [12, 14, 15]. This study aims to build on current efforts by making a computational model of a hydrogen retrofit of the ATR 72-500. The specific use of hydrogen is later discussed. An example of an ATR 72 with a hydrogen fuel tank can be seen in Fig. 1.

There are two prevalent hydrogen propulsion technologies: electric propulsion via hydrogen Fuel Cells (FC), and the direct combustion of hydrogen. Although there have been recent breakthroughs in the hydrogen FC technology [16], there is still uncertainty regarding the systems surrounding the FC, such as cooling [17]. The overall performance of the FC and these surrounding systems will determine whether the extent to which the technology is viable for aircraft applications. Hydrogen combustion, on the other hand, is known to work; the HeS 1 Demonstrator Engine, a predecessor to the first jet engine ever flown, used hydrogen [18]. For this reason, this study has chosen to investigate hydrogen combustion.

In order to minimise the time required for hydrogen combustion to be implemented, hybrid aircraft must be considered. Similar to what is being done with SAF-kerosene blends, hybrid aircraft do not necessarily rely on the new technology, meaning that its certification can happen in stages as opposed to in one go. If this were to be allowed, the potential benefit is twofold: some of the emissions reductions of hydrogen can be already claimed, and designer understanding of the technology can be faster increased. In the literature, hydrogen-electric hybrid aircraft [19] and kerosene-electric hybrid aircraft [20] have already been considered, however not many efforts have been made towards investigating hydrogen-kerosene hybrid aircraft. This investigation aims to contribute towards covering this gap in the literature by making a computational model of a hydrogen retrofit of an ATR 72-500 with engines capable of combusting a hydrogen and kerosene fuel blend.

The assumption that such engines can be made is based on three studies. In an investigation performed in 1980, kerosene-hydrogen combustion was successfully performed in a gas turbine combustor for a proportion of hydrogen ranging from 0-100% [21]. The combustor used consisted of a hybrid fuel nozzle, a swirler, a combustion liner with holes for secondary air, and an exhaust duct. A diagram of a hybrid fuel nozzle similar to the one used in [21] is available in Fig. 2. With this, the combustion properties of the mixture were characterized. When 10-50% hydrogen was used, higher efficiencies and lower NO_x emissions were obtained and, when over 50% of hydrogen was used, the flame properties resembled that of hydrogen. The hydrogen doping approach is also being investigated for the UK gas network as part of the UK hydrogen strategy [22], which could lead to technology transfer to the aerospace sector. A more recent computational study on hybrid combustion in a gas turbine combustor found that NO_x levels beneath 1 ppm could be obtained at 30% hydrogen [23]. Finally, a hybrid engine concept has been modelled and analysed as part of the AHEAD project in TU Delft [24]. Unlike the other investigations, this concept uses two separate combustion chambers for hydrogen and kerosene, and introduces new technologies to the turbofan engine. Such technologies include using hydrogen for bleed air cooling and a contra rotating fan. Reductions in both CO_2 and NO_x were also obtained with this new concept. With hydrogen doping being currently possible in gas turbine combustors, and improvements to the technology already being considered, analysing a hybrid combustion retrofit is justified.

As the ATR 72 is an aircraft originally designed for kerosene, introducing hydrogen will mean that the retrofit will operate off-design and will hence be sub-optimal. Designing such a retrofit will require exploring the hydrogen aircraft design space, which is not currently very well understood. To avoid the baked-in biases towards kerosene designs from both the designer and the first-order aircraft design methods, abstraction is needed. This abstraction can be provided by using an optimization approach to the retrofit. However, defining a suitable objective function for an aircraft design is non-trivial due to the large number of performance metrics available. Further, the relative importance of the objectives might not necessarily be constant or quantifiable. To address these issues, this investigation will use Multiple Dominance Relations (MDR) [25] within the optimization routine. With this, the goals of the study can now be summarised:

- 1) To bring understanding of the hydrogen-kerosene combustion design space and approximate the fundamental trade-offs in it.
- 2) To extract order-of-magnitude estimates for the performance of future hydrogen aircraft designs.
- 3) To provide a potential pathway for the full adoption of hydrogen-powered aircraft via kerosene-hydrogen hybrid retrofits.

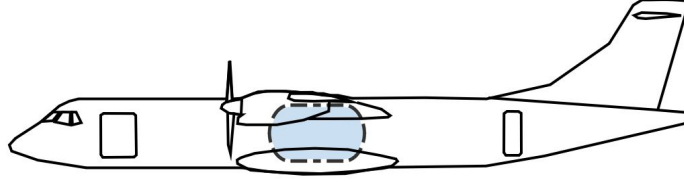


Fig. 1 A wire sketch of the ATR 72 reconstructed from [26]. The blue shape with a dashed outline represents a hydrogen tank. The tank is not to scale.

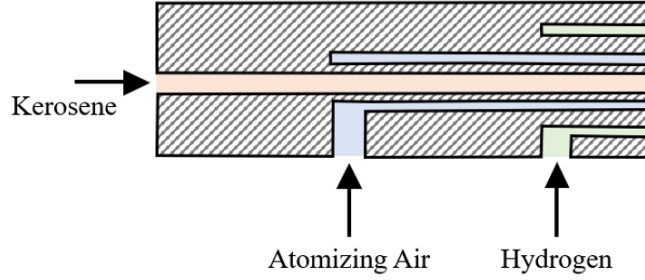


Fig. 2 A reproduction of the diagram of the hybrid fuel nozzle used in [21].

III. Methods

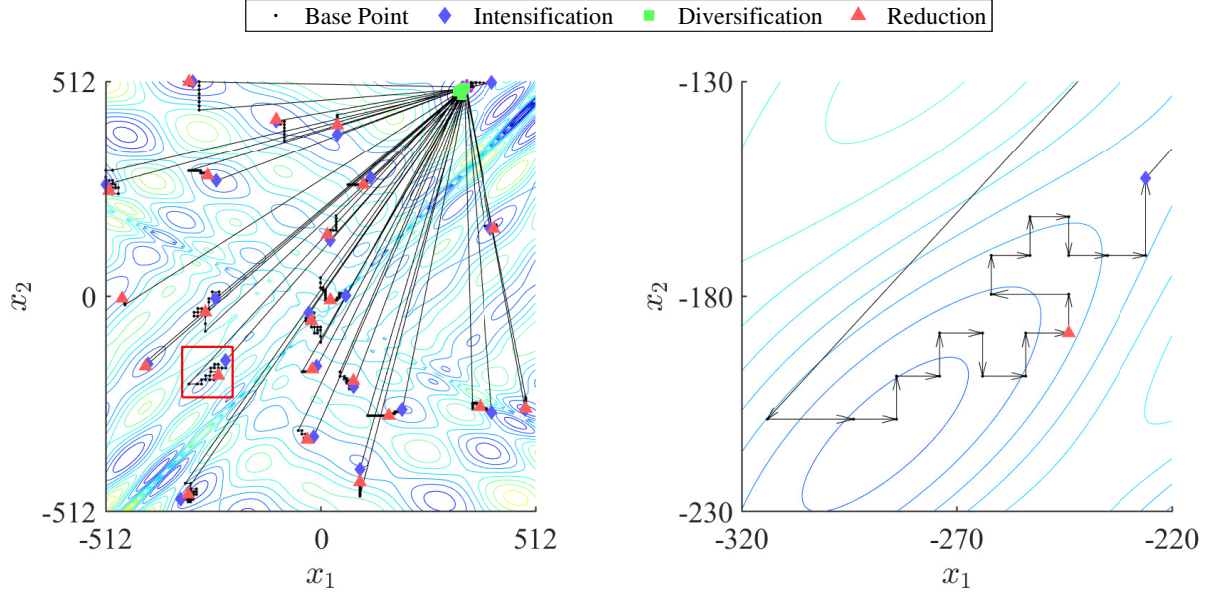
A. Optimization

1. Search Algorithm

The aircraft design space is very fragmented due to the presence of both discrete and continuous variables. Only *pattern search* algorithms, *population* algorithms, or modified *stochastic* algorithms are able to handle such a design space. However, neither population nor stochastic algorithms offer the designer insight as to how decisions are being made real-time. This is unacceptable for the aviation industry due to the stringent levels of validation required for safety purposes. One pattern search algorithm that is able to navigate the fragmented design space in a way that is understandable, justifiable and traceable for a designer is Tabu Search (TS) [27]. For this reason, TS has been chosen as the search algorithm for this endeavour. To navigate such a fragmented design space, TS makes use of three basic movements:

- 1) **Local Search:** A modified Hooke-and-Jeeves local search is used [27]. This consists of moving on a grid of a pre-determined step size and comparing the current point (base point) with the neighbouring points. The best improvement to the objective function is chosen as the next base point. This best improvement can also be negative when no positive improvement is available, allowing the algorithm to climb out of local minima. The local search uses a short-term memory to prevent re-visiting points.
- 2) **Intensification:** The search is moved near a promising region of the design space. The specifics of this movement vary between implementations, but they involve the use of a medium-term memory or an intensification memory to store promising points.
- 3) **Diversification:** The search is moved to an under-explored region of the design space. This is done by keeping a tally of how many times the different regions of the design space have been visited in a long-term memory.

Both intensification and diversification occur after there are INTENSIFY and DIVERSIFY consecutive movements which do not improve the objective function. INTENSIFY and DIVERSIFY are constants chosen by the designer. Figures 3a and 3b provide a visualization of the Tabu Search used to optimise the 2D eggholder function. The eggholder function contains many local minima and maxima, making it appropriate for visualising the TS search pattern. It is also a standard benchmark in optimisation literature [28]. Full details of the basic TS implementation can be found in [27].



(a) TS search pattern over the range $|x_i| < 512$ for $i = 1, 2$. There are 200 objective function units between each contour. The closer the contours are to dark blue, the lower the objective function value. (b) Enlarged boxed region from Fig. 3a, showing local search just after a diversification step. The optimiser reaches a local minima and then leaves its region of influence. There are now 100 units between each contour.

Fig. 3 TS search pattern for the 2D eggholder function.

2. Comparison of Designs Using Multiple Dominance Relations (MDR)

Consider an aircraft design x that lies in the feasible aircraft design space $\mathbb{X}$. The performance of the aircraft is evaluated by an objective function $f(x)$, which maps $\mathbb{X}$ to the performance space $\mathbb{Q}^m$ such that $f(x): \mathbb{X} \rightarrow \mathbb{Q}^m$. This performance space consists of m objectives to be minimised. Comparing the performance of different designs is non-trivial for $m > 1$. For this, a binary relation (denoted by $\leq$) can be defined such that a design $x \in \mathbb{X}$ dominates another design $y \in \mathbb{X}$ if $x \leq y$. With this, the set of optimal designs in $\mathbb{X}$ with respect to a binary relation can be defined, and is denoted by $\min(\mathbb{X}, \leq)$ [25]:

$$\min(\mathbb{X}, \leq) := \{x \in \mathbb{X} \mid \nexists y \in \mathbb{X} \text{ for which } y \leq x \cap x \not\leq y\} \quad (1)$$

In Multi-objective Optimization (MO), a candidate design $x \in \mathbb{X}$ dominates another design $y \in \mathbb{X}$ if all m objectives in x are strictly smaller than the corresponding m objectives in y . This is known as Pareto dominance, and is denoted by $x \leq_{\text{Pareto}} y$ [25, 29].

$$x \leq_{\text{Pareto}} y \Leftrightarrow f_i(x) < f_i(y) \quad \forall i \in 1, \dots, m \quad (2)$$

Similarly, a pair of designs is Pareto equivalent if neither design Pareto dominates each other ($x \not\leq_{\text{Pareto}} y$ and $y \not\leq_{\text{Pareto}} x$). The Pareto front consists of the performance vectors of the optimal designs according to $\leq_{\text{Pareto}}$, and is denoted $\text{PF}(\mathbb{X})$ [25]:

$$\text{PF}(\mathbb{X}) := \{f(x) \in \mathbb{Q}^m \mid \nexists y \in \mathbb{X} \text{ for which } y \leq_{\text{Pareto}} x \cap x \not\leq_{\text{Pareto}} y\} \quad (3)$$

This can be thought of as the hyper-surface which contains all fundamental trade-offs present in the design problem. The greater the number of objectives m , the greater the number of designs in the Pareto front. The higher dimensionality of the hyper-surface therefore makes it harder for an engineer to understand the fundamental trade-offs in this design problem. A higher the number of designs in the Pareto front also makes it harder to discriminate between the better and worse designs manually which is a requirement for the aerospace industry. With a large number of objectives in aircraft design, an alternative approach is required to discriminate between candidate designs.

The alternative proposed in [25] is known as Multiple Dominance Relations (MDR). The key concept behind MDR is to use n nested binary relations instead, finding sets of optimized designs *within* sets of optimized designs [25]:

$$\mathbb{X}_{\text{optimal}} := \min(\dots(\min(\min(\mathbb{X}, \leq_1), \leq_2) \dots), \leq_n) \quad (4)$$

In this study, each of the binary relations in Eq. (4) is defined as Pareto dominance (Eq. (2)) for only two objectives at a time. For this, an ordered list of objective pairs must be provided to be used as the objectives in Eq. (2) at each layer. Each of these objective pairs is known as a *dominance layer*. Computing the Pareto front for a given dominance layer is done by assigning a rank $\hat{R}_k(x)$ to each design in the set of candidate designs $\hat{\mathbb{X}}$, where $\hat{\mathbb{X}} \subset \mathbb{X}$. See Algorithm 1 for more details on how these ranks are assigned. The set of designs with the lowest rank are those whose performance lies on the Pareto front.

MDR is advantageous over MO because the order of the dominance relations affects the outcome and thus can be used to reflect the relative importance of the performance metrics. To obtain results with desirable attributes, the most important objectives are put in the top dominance layers, with the relative importance of these objectives decreasing with an increasing layer number [30]. This allows for the majority of trade-offs to be done automatically in a way that is understandable for the designer, leaving a manageable amount of designs to consider manually. This ranking method has been previously used with Tabu Search, and the results show that it outperforms other methods [31].

Algorithm 1 Finding the rank of a set of designs according to the k -th binary relation $\leq_k$. Adapted from [25].

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1: procedure FINDRANKS( $\hat{\mathbb{X}}, \leq_k, \hat{R}_k$ )
2:   for  $x_i \in \hat{\mathbb{X}}$  do
3:     count  $\leftarrow$  0
4:     for  $x_j \in \hat{\mathbb{X}}$  do
5:       if  $x_j \leq_k x_i$  and  $x_i \not\leq_k x_j$  then
6:         count = count + 1
7:       end if
8:     end for
9:      $\hat{R}_k(x_i) \leftarrow$  count
10:  end for
11: end procedure

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3. Performance Metrics

With numerous ways to characterize the performance of aircraft, the choice of objectives must be limited. In this study, four metrics have been chosen: the CO_2 emissions per Revenue Passenger Kilometer (RPK), the fuel energy per RPK, the payload weight proportion, and the L/D .

The emissions metric was chosen since the legislative goals are defined in terms of it. This metric measures the mass of CO_2 produced by the engines exclusively. It does not include any embedded emissions from the production, transport, and storage of the fuels. It also does not account for the NO_X produced by the engine, nor does it include the radiative forcing effects of the contrails produced by the aircraft.

The energy metric was chosen as a proxy for cost since it is the key driver of the market. Though not proportional to the mission energy, the cost is a monotonically increasing function of the mission energy since both functions are linear combinations of the on board fuel masses. Therefore, some of the trends in cost can be captured by the energy requirements. As with the emissions, the energy metric only accounts for the chemical energy that can be extracted from the fuel at the engines, neglecting any energy required to produce, transport, and store the fuels.

The payload proportion was chosen as one of the metrics to be used due to its significance in real-world applications. No major airline would be willing to purchase an aircraft that is carbon-neutral but can carry very few passengers due to its high operating costs per passenger, and its inability to fulfill demand. Including this as a metric will force the optimizer to look for aircraft that are both better environmentally and practically.

The L/D was chosen as the final metric to force the optimizer to find a suitable operating point for the aircraft. This metric ensures that the optimizer will not propose hydrogen aircraft with a sub-optimal operating point but good emissions.

4. Description of the Optimization Runs

The optimization runs in this study use two dominance layers. For each run, the important metrics were placed in the top dominance layer (see Section III.A.2). The relative importance of each metric depended on the purpose of each optimization run. Note that all runs performed in this experiment consisted of a maximum of 1200 aircraft evaluations

each. The optimization run could also finish if all variables reached the minimum step size.

For the hybrid optimisation accounting for the current needs, the emissions per RPK and the payload proportion were placed in the first layer, whereas the mission energy per RPK and the L/D were placed in the second layer. This order reflects the current need to decrease emissions in a way that is not too costly. If there were more than one member of the second-layer Pareto front, the optimized design was defined as that with the least energy use per RPK. The remaining designs, if any, were manually considered.

As the current deadline to reach net-zero is approached, the emissions of the aircraft per RPK will become an increasingly important metric. The previously established objectives will therefore no longer be representative of the industry needs. This is addressed by undertaking a final optimisation in which the L/D is replaced by the emissions per RPK in the second dominance layer of the initial hybrid optimisation. If the second-layer Pareto front was populated with more than one design, the optimized design was chosen to be that with the least emissions per RPK in this final run, as opposed to the design with the least energy per RPK chosen in the previous runs. Once again, the remaining designs, if any, were manually considered.

Validation of the above optimization runs has been performed with another optimisation. This consisted of optimising an aircraft designed for the same range without using hydrogen. This run starts from the same design point as the *current needs* run and uses the same seed, meaning that the performance benefits from this run can be attributed to non-hydrogen effects.

Further validation has been conducted. First, an evaluation of the ATR 72 model has been performed at the standard mission (defined in Section III.D) as an additional benchmark. Secondly, the aircraft model has also been evaluated at 1000 evenly spaced values of Φ_{H_2} whilst keeping all the other parameters constants to identify the effects of hydrogen.

B. System Architecture

Figure 4 provides a high-level view of the architecture of the system and the information flow between the function carriers. First, TS provides the aircraft model with a candidate aircraft design. The aircraft model is then evaluated, which runs two simulations in X-Plane 11 [32] and produces the performance metrics for the aircraft. By storing the previous performances, MDR can then rank the new design relative to the existing designs. This ranking allows TS to generate a new candidate design based on the information of the past designs.

The simulator has two roles within this architecture. Firstly, it can be used to minimise the use of correlations from literature, which are likely to have baked-in biases towards kerosene. The simulator can also be used to improve estimates and to validate data by checking whether a particular aircraft design can actually sustain its design cruise point (see Section III.E). The optimiser communicates with X-Plane 11 by transmitting data using UDP (a standard communications protocol) over a LAN. In this investigation, a modified version of X Plane Connect (XPC) [33], an X-Plane 11 plugin, was used in order to handle the communications.

C. Aircraft Model

A visual representation of the aircraft model has been provided as a modified Functional Analysis Systems Technique (FAST) diagram (Fig. 5). Figure 6 has also been given in order to understand the inputs and outputs of the system.

Since W_0 and L/D are both inputs and outputs of the aircraft model, the aircraft design process must be iterative. As aircraft simulations in X-Plane 11 are very computationally expensive, it has been decided that no more than two iterations should be done per aircraft evaluation. The first of these iterations uses an L/D estimate obtained from Raymer [34] and assumes that W_0 is the ATR 72-500 MTOW. Although two iterations do not result in convergence, they are sufficient to capture the trends to a first-order.

Discarding the variables which act as both inputs and outputs, as well as the range (which is fixed), the optimiser navigates the design space formed by the following variables and their corresponding feasible ranges:

- 1) Maximum single engine power ($1500 \leq P_{max} \leq 3500$ kW)
- 2) Cruise Altitude ($14\,800 \leq h \leq 25\,000$ ft)
- 3) Cruise Mach Number ($0.4 \leq M \leq 0.67$)
- 4) Hydrogen power fraction ($0 \leq \Phi_{H_2} \leq 1$)

The feasible range for the engine P_{max} was chosen to guarantee interpolation in the engine correlations (Figs. 7 and 8), and the range for h was chosen so as to not violate the base operational ceiling of the ATR 72 (25000 ft according to its type certificate [35]). The range for M was chosen from personal experience, and the range for Φ_{H_2} follows from its definition. The initial parameter values for all optimisation runs are as follows: $P_{max}|_0 = 2050$ kW, $h|_0 = 20\,000$ ft, $M|_0 = 0.45$, and $\Phi_{H_2}|_0 = 0.5$ (except for the kerosene-only run where $\Phi_{H_2} = 0$ always).

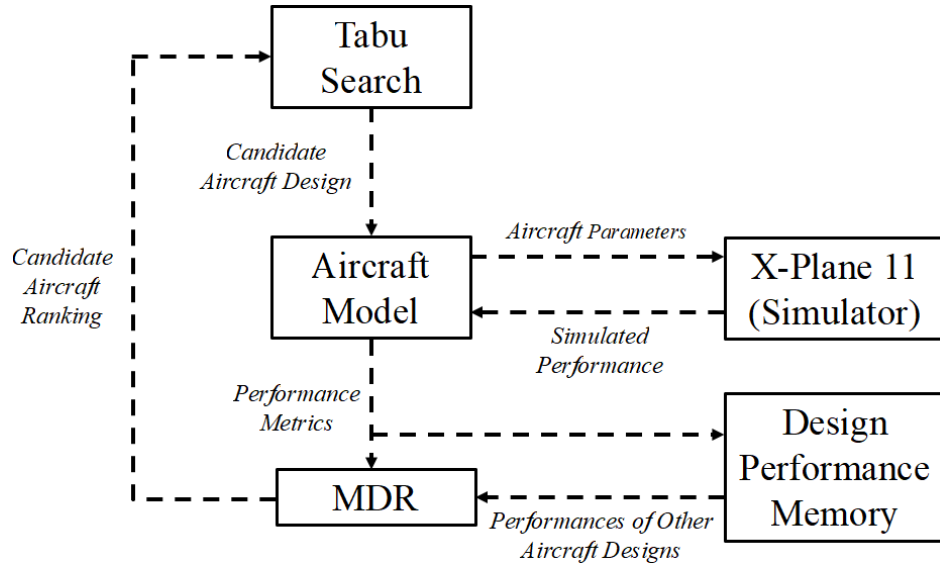


Fig. 4 Diagram showing the high-level architecture of the chosen optimiser and objective function. The dashed arrows indicate information flow. The text in italics indicates the type of information, and each blocks represents a function carrier.

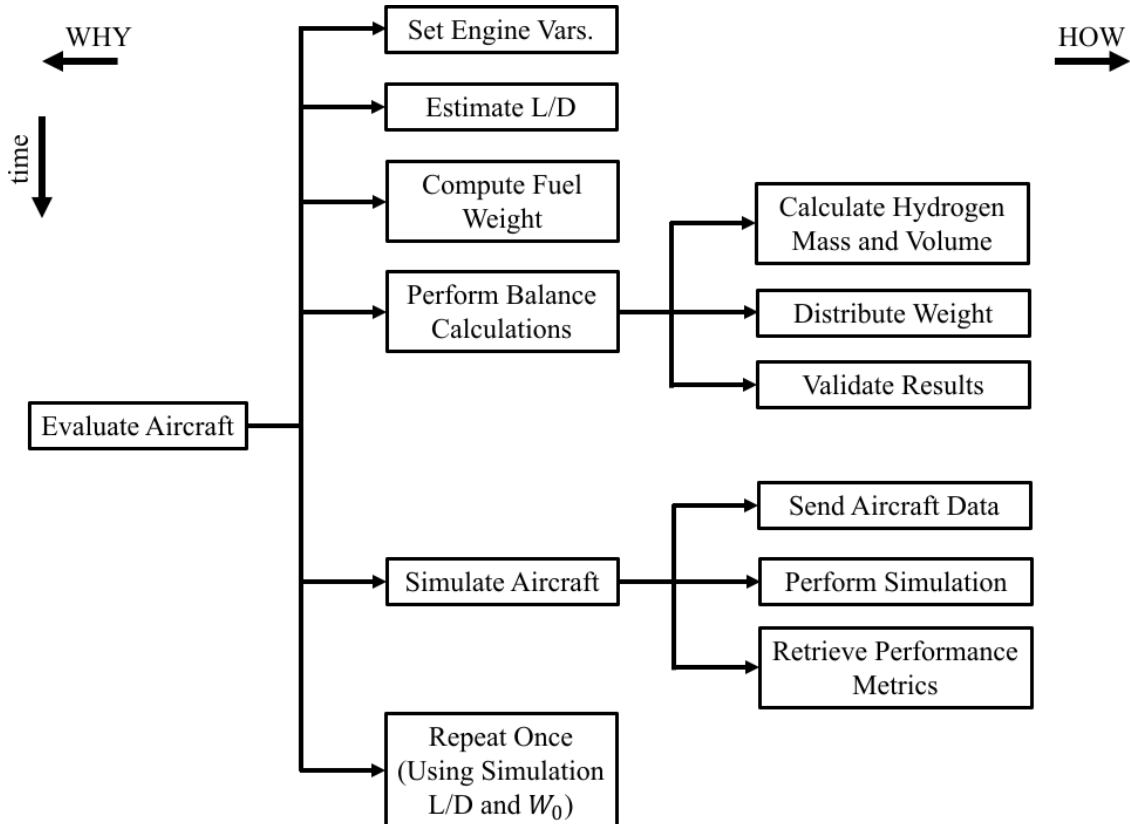


Fig. 5 Modified Functional Analysis Systems Technique (FAST) diagram for the aircraft model.

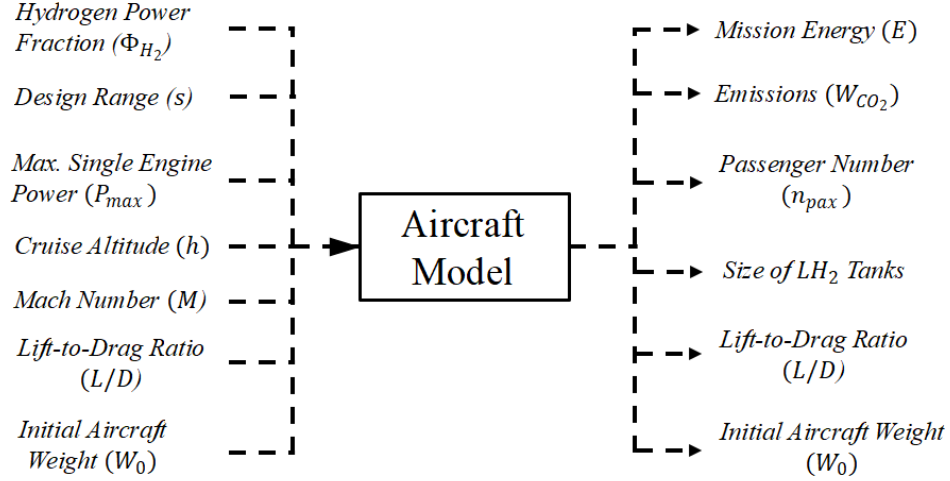


Fig. 6 Diagram showing the inputs and outputs of the aircraft model. The dashed arrows indicate information flow. The text in italics indicates the type of information. The inputs lie to the left of the main block, and the outputs to the right of it.

1. Engine Model

To model the change in fuel consumption and mass of the engines with rated engine power, data from the PW100 engine family has been used to make correlations for a rubber engine model (Figs. 7 and 8). The change in engine performance with altitude has been modelled using the publicly available Flight Crew Operating Manual (FCOM) of the ATR 72. To account for the hydrogen, calculations from first-principles have been used (see the Appendix). The key relation obtained is given here:

$$BSFC = \frac{1}{\eta_{th}} \cdot \left[\frac{1}{C_{H_2}} \cdot \Phi_{H_2} + \frac{1}{C_{JA1}} \cdot (1 - \Phi_{H_2}) \right] \quad (5)$$

Where Φ_{H_2} is the hydrogen power fraction (or hybridisation fraction), η_{th} is the engine thermal efficiency, and c represents the specific energy of the relevant fuel.

The derivation of this equation makes two assumptions: that hydrogen and kerosene can be combusted together, and that the thermal efficiency stays constant. The former assumption is validated by the successful endeavour in which hydrogen and kerosene were burnt together in a gas turbine combustor [21]. The latter assumption is validated by the fact that gas turbine thermal efficiencies are currently limited by the turbine entry temperature [36].

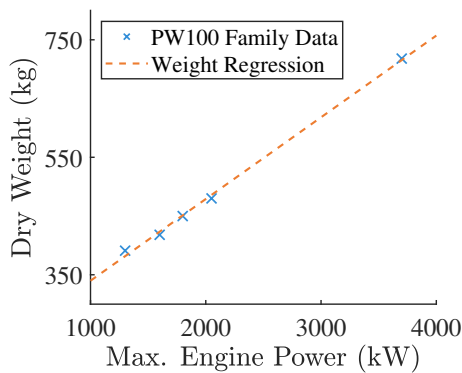


Fig. 7 Correlation between the engine dry weight and the maximum engine power for the PW100 family. The correlation is given by: $\text{Weight (kg)} = 0.1391 \cdot \text{Power (kW)} + 200.75$. Data from [37, 38].

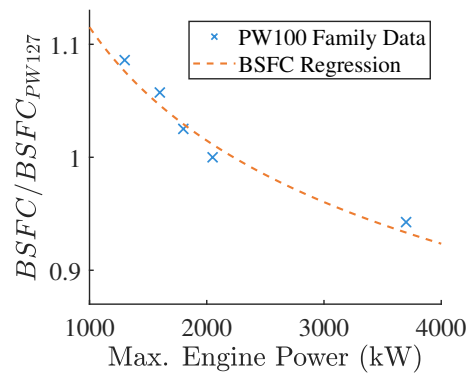


Fig. 8 Correlation between the $BSFC$ factor and the maximum engine power for the PW100 family. The correlation is given by: $BSFC/BSFC_{PW127} = 2.853 \cdot [\text{Power (kW)}]^{-0.136}$. Data from [37, 38].

2. Liquid Hydrogen Storage

The liquid hydrogen tank model has been formed with data from [39] exclusively. These tanks are comprised of elliptical cylinders with curved end-caps, and the definitions of their geometric variables can be seen in Fig. 9. A new efficiency metric is defined in [39], which is given by the following expression:

$$\eta_{req} = \frac{W_{H_2 req.}}{W_{H_2, net} + W_{tank}} \quad (6)$$

Where η_{req} is the storage efficiency of the tank, $W_{H_2 req.}$ is the required amount of hydrogen to perform the flight, $W_{H_2, net}$ is the total weight of hydrogen (including the gaseous fraction required for venting and pressure control), and W_{tank} is the weight of the hydrogen tank.

The hydrogen tank used in this investigation assumes the same design point as the example given in [39]. Here, it was shown that the storage efficiency of the tank is not very sensitive to changes in the length ratio λ if $\phi \approx 1$. Besides the fact that all fuselage shapes of commercial aeroplanes are effectively cylindrical, it was deemed appropriate to choose $\phi = 1$, making $\eta_{req} \approx 0.63$ regardless of the length ratio of the cylinder. The remaining parameter was fixed to $\psi = 1$.

With the fill pressure being 1.2 bar, and the venting pressure being 1.448 bar, $\rho_{LH_2} = 69.2 \text{ kg/m}^3$ and $f \approx 0.93$ [39] the internal tank volume is calculated as follows:

$$V_{H_2, net} = \frac{W_{LH_2}}{\rho_{LH_2} \cdot f} \quad (7)$$

The internal length of the tank can thus be calculated from the internal volume and the maximum allowed tank radius r_{max} :

$$l_t = \begin{cases} \left(V_{H_2, net} - \frac{4}{3}\pi r_{max}^3 \right) / \pi r_{max}^2 + 2r_{max}, & \text{if } V_{H_2, net} > V_{sphere, max} \\ 2 \cdot (3V_{H_2, net} / 4\pi)^{1/3}, & \text{otherwise} \end{cases} \quad (8)$$

Where $V_{sphere, max}$ is the volume of a sphere with radius r_{max} .

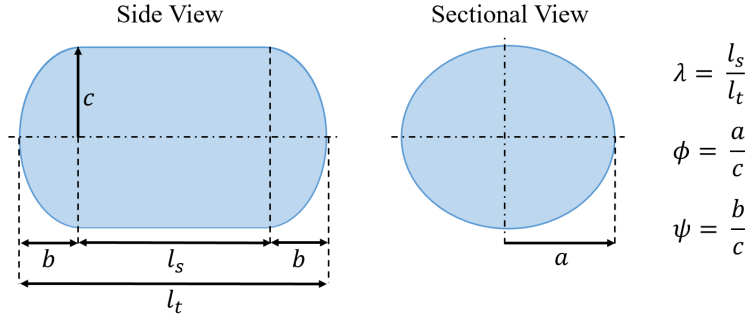


Fig. 9 Definition of hydrogen tank dimensions. This figure has been reconstructed from [39].

3. Weight and Balance

The weight and balance calculations in the aircraft model are done sequentially. First, the engine correlations from Section III.C.1 are used to calculate the delta in engine weight. Since MTOW is the limiting weight and is determined by the undercarriage and fuselage (which remain unchanged in this investigation), it is constant for a retrofit and hence its value is equal to that of the ATR 72. With this, the empty weight less the hydrogen tank mass is computed.

Next, the MTOW can be used to calculate the net fuel mass required for the mission (specified in Section III.D). The mass of each fuel can now be calculated with the following expression, which has been derived in the Appendix:

$$W_{H_2 req.} = W_{fuel, net} \cdot \left[1 + \frac{C_{H_2}}{C_{JAI}} \cdot \left(\frac{1}{\Phi_{H_2}} - 1 \right) \right]^{-1} \quad (9)$$

The kerosene is placed in the fuel tanks of the ATR 72, which are located in the wings. The mass of the hydrogen storage system is found from Eq. (6), and the length of the tank is found using Eq. (8).

To ensure that the centre of mass of the empty aircraft does not move significantly, the hydrogen tank is placed coincident to the centre of mass of the empty aircraft, which lies roughly in the centre of the cabin (Fig. 1). This strategy assumes that the passenger cabin can be split in two. The tank length is then used to calculate the number of seats that need to be removed due to the presence of hydrogen. The maximum number of passengers is the lowest admissible from either the un-allocated weight to reach MTOW or the number of seats available.

The average passenger mass, including any small carry-on, is taken as 80 kg/pax. This is beneath the recommended value by the European Union Aviation Safety Agency (EASA), 84 kg/pax [40]. The reduction in mass follows from the assumption that some of the large carry-on items will go in the cargo hold due to the small size of the cabin. The passengers are distributed symmetrically between the front and rear cabins to keep the centre of gravity within its feasible range. The remaining weight is assumed to be cargo, filling the front hold followed by the rear hold. This order was chosen since the empty centre of gravity of the aircraft already lies somewhat close to the aft limit.

D. Flight Envelope and Fuel Weight

This project aims to provide a flight profile that is accurate to a first-order. The minimum flight profile was determined to consist of take-off, climb, cruise, descent, and landing. To enable the comparison of results between different aircraft, a standard mission has been specified. It is defined as an aircraft flying a range of 750 km at its optimal cruise height and speed, with its maximum possible take-off weight. The choice of this range is justified in the next section.

1. Cruise and Cruise Range

For a retrofit with hydrogen in the cabin, it is necessary to make the range of the aircraft as low as is feasible. This is because higher ranges require higher masses of hydrogen, which results in less passengers being able to fly. With 90% of ATR 72 flights in 2019 being under 750 km [41], a design range of 750 km has been chosen for this investigation.

In this experiment, cruise has been modelled to occur at a constant cruise altitude and speed. It has also been assumed that the lift-to-drag ratio of the aircraft is constant. This means that, for each configuration, the aircraft can be placed in the simulator at its cruise conditions to extract some of the performance metrics. The Breguet range equation is then used to obtain a first-order approximation for cruise fuel weight:

$$s = \frac{\eta_{prop}}{g} \frac{1}{BSFC} \frac{L}{D} \ln \left(\frac{W_0}{W_f} \right) \quad (10)$$

Where W_0/W_f is the ratio of start-of-cruise to end-of-cruise aircraft weights.

2. Climb and Descent

Validated first-order models for climb and descent have been used from the Techno-Economic Analysis of Aircraft (TOSCA) project [42]. For climb, an energy-based method is used between lift-off and the top of climb in which the drag force is constant. This is achieved by assuming a constant climb angle β and a constant lift-to-drag ratio $(L/D)_{av}$ throughout the climb:

$$\begin{aligned} \Delta E_{climb} &= \Delta KE_{climb} + \Delta PE_{climb} + (Dw)_{climb} \\ \text{with } (Dw)_{climb} &\approx W_{liftoff} \cdot \frac{gh \cot \beta}{(L/D)_{av}} \end{aligned} \quad (11)$$

Where E is the work done, KE is the kinetic energy, PE is the gravitational potential energy, D is the drag force, w_{climb} is the climb distance, and $W_{liftoff}$ is the mass of the aircraft at liftoff. For this model, $\beta \approx 3.2^\circ$. Throughout both climb and descent, $(L/D)_{av} = 15.7$ [42].

Similarly, the descent model is also emulated from [42]. This uses an energy method that assumes that the aircraft is in gliding flight, descending at a constant True Airspeed (TAS) at an angle given by $\tan \theta_d = [(L/D)_{av}]^{-1}$. The work done during descent can be considered a factor f times the work done during cruise:

$$\Delta E_{descent} \approx f \cdot W_{cr-end} \cdot \frac{gh}{(L/D)_{av} \sin \theta_d} \quad (12)$$

Where W_{cr-end} is the mass of the aircraft at the end of cruise, and $f = 0.9$ for the ATR 72-500 [42].

Since the $BSFC$ is inversely proportional to the thermal efficiency η_{th} (Eq. (5)), Eqs. (11) and (12) can be used alongside the definition of the $BSFC$ to calculate the climb and descent fuel masses for a hybrid aircraft:

$$m_{fuel} = \left(\frac{BSFC}{\eta_{prop}} \right) \cdot \Delta E \quad (13)$$

Where the quantity $BSFC/\eta_{prop}$ can be computed from a modified Eq. (5), replacing η_{th} with η_{ov} . A value of $\eta_{ov} = 0.255$ is given for both climb and descent in the ATR 72-500 [42].

3. Take-Off

The take-off model is developed in-house. A constant acceleration is assumed from a standstill to the minimum flight speed V_2 . This is used in combination with real data for the take-off distance and its corresponding engine power to provide the mass of fuel consumed. The engine power, V_2 , and take-off length are 1845 kW, 115 kt, and 1404 m respectively [43]. The time required for the take-off run can then be calculated, which can then be used with an estimate for the $BSFC$ to compute the mass of fuel burnt at take-off. To estimate the hybrid $BSFC$ at take-off, η_{th} is taken to have a value of 0.27. This approximately corresponds to the worst η_{th} derived from the ATR 72 FCOM.

4. Eventualities

ICAO Annex 6 Section 3.4.3.5.3 states that, other than the planned trip fuel, an aircraft must load fuel for eventualities [44]. For this experiment, only contingency fuel and final reserve fuel are considered. The contingency fuel is to be no less than 5% of the planned trip fuel [44]. However, the final reserve fuel for turbine-engined aircraft is defined in terms of elevation above the airport. In this exercise, the final reserve fuel for requirement for aircraft with reciprocating engines is chosen instead. This states that the aircraft must be able to fly for 45 additional minutes after it has landed [44]. Note that this implies that the final reserve fuel is not burnt on a typical flight, and so will not be accounted for when computing the emissions and mission energy. It will, however, be carried in the aircraft so the tanks are sized with it in mind. The additional flight time has been assumed to take place at cruise conditions.

E. Real-Time Verification Strategies

Part of what makes aircraft design difficult is that the unfeasible regions are not necessarily known *a priori* of the evaluation of the aircraft model, and that these regions are functions of multiple variables. For example, an engine might be under-powered to cruise at a certain Mach number. In the simulation, the aircraft is instantaneously placed at the design cruise altitude at the design cruise speed so the optimiser is not able to tell immediately whether the unfeasible region is reached. Care must be taken to verify that the aircraft is feasible in practice. The following list indicates the ways in which an aircraft can be unfeasible with all of its variables lying in their individual feasible spaces:

- 1) The total calculated mass is greater than MTOW.
- 2) The hydrogen tanks do not fit in the aircraft.
- 3) The aircraft cannot maintain the design cruise point.
- 4) The aircraft has its Centre of Gravity (CG) outside of its certified envelope.

The first two issues only require a check to see whether the total mass is greater than MTOW, and another check to see whether the tank can fit within the fuselage. The third issue has been circumvented by comparing the desired and measured operating point variables. Specifically, the optimiser checks whether the measured TAS and the cruise altitude lie within 5% of the demanded values. The vertical speed of the aircraft is also checked, with its magnitude needing to be below 100 ft/min for the aircraft to be considered feasible.

The fourth issue is also hard to deal with due to the low quality of the publicly available load and balance sheets for the ATR 72. This requires estimation in the location of the CG of several components. In addition, there are many possible re-arrangements of the load possible for the aircraft, some of which result in an acceptable CG location and some that do not. For these reasons, using the take-off and landing CG limits has been deemed inappropriate. Instead, the in-flight CG limits for the aircraft have been used, which are more generous. With this, a rough estimate can be made as to whether the aircraft is flyable or not.

Finally, given that the optimiser communicates with X-Plane 11 via UDP, it is possible that packet loss can occur. In order to prevent receiving erroneous data, XPC warns the user and discards the received data when there is a communication problem. The optimiser therefore makes any planes that were subject to packet loss infeasible. The

infeasible planes are not discarded, but they are rather given performance metrics with physically unattainable values that make these designs undesirable when considered by MDR. These designs do not feature in the results.

IV. Results and Discussion

A. The Effects of Hydrogen

In order to understand the effects of hydrogen on the retrofit, 1000 aircraft models have been in which only Φ_{H_2} was varied. These runs did not use the simulator, since their purpose is to characterize the in-house model. For this, a constant L/D equal to that obtained for the simulation of the baseline ATR 72 model was assumed. The effects of the hybridisation fraction on the emissions and energy per RPK have been documented in Figs. 10 and 11 respectively, and the corresponding number of passengers have been documented in Fig. 12.

Figure 10 shows that increasing the proportion of hydrogen generally results in a decrease in the emissions per RPK. This is expected as no emissions are attributed to hydrogen production in this model. The instances where this trend is not followed correspond to a sudden decrease in the number of passengers that results from a row of seats being removed to make space for the hydrogen tank (Fig. 12). The manner in which emissions decrease with Φ_{H_2} is not as anticipated — It was thought that the increase in emissions per passenger would have significantly increased with Φ_{H_2} . In practice, however, this increase is limited because the number of passengers is still large (Fig. 12). This means that the factor proportional to $1/n_{pax}$ in the emissions per RPK still lies in the region with a low gradient, so changes to the number of passengers have a low impact on the emissions. This can be observed in Fig. 11, where the difference between the large linear regions appears to grow slowly with Φ_{H_2} . Furthermore, in Fig. 10 this effect is enhanced by the fact that the emissions decrease faster with Φ_{H_2} than the $1/n_{pax}$ factor increases, resulting in a limitation to the adverse effects of removing passengers. This suggests that the available improvements in emissions for the optimiser to make relative to a straight retrofit will also decrease with Φ_{H_2} .

In the linear regions, the energy per RPK exhibits a small negative gradient, which can be neglected for the purposes of the subsequent analysis. Another noteworthy feature is the presence of jumps prior to the step increases in Fig. 11. It was previously indicated that aircraft design is an iterative process, and that this model only performs two iterations. Close to a change in the number of passengers, the iterations jump back and forth between having and removing a row of passengers. Figure 12 has some evidence for this: the last vertical line is thicker than the others, suggesting the presence of multiple jumps. Consider now the scenario in which the first iteration assumes that the number of passengers decreases, whereas the second iteration assumes that the number of passengers increases. The weight used to compute the fuel of the second iteration is lower, corresponding to that of an aircraft that carries one row less of passengers. In practice, when computing the energy per RPK in the second iteration, the lower amount of fuel is divided by a larger number of passengers than it should, resulting in the decrease observed in Fig. 11 (and in Fig. 10 to a much lesser extent). The converse can also occur, leading to an increase in the relevant metrics per RPK observed in the same figures. In practice, these effects combine, appearing as spikes. Due to the ambiguity, designs that lie in these regions should be considered to have the emissions and energy values of the next linear region.

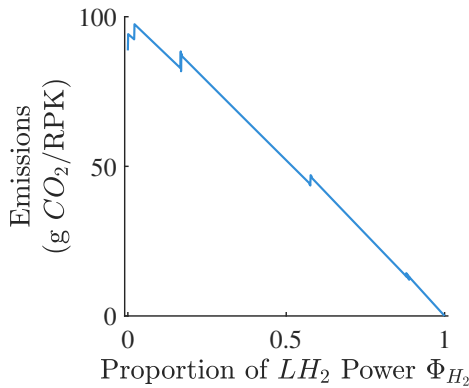


Fig. 10 Effect of hybridisation on emissions for a straight retrofit of the ATR 72-500 flying the standard mission.

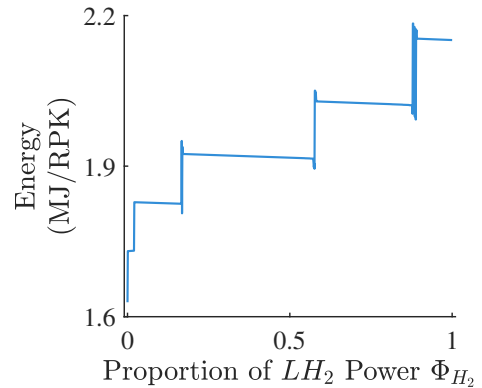


Fig. 11 Effect of hybridisation on the mission energy for a straight retrofit of the ATR 72-500 flying the standard mission.

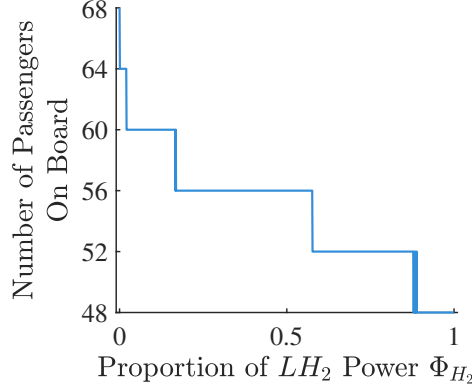


Fig. 12 Effect of the hybridisation fraction on the maximum number of passengers on board for a straight retrofit of the ATR 72-500 flying the standard mission.

B. Hybrid Optimization

1. Hybrid Optimisation for Current Needs

For the optimisation accounting for current needs, the first and second layers of the design performances can be found in Figs. 13 and 14.

Figure 13 shows that most designs are, within their clusters, concentrated towards the bottom-left. This suggests that the optimiser has successfully discriminated between good and poor designs. This Pareto front reveals the trade-off between the payload fraction and the amount of emissions. This is to be expected since adding hydrogen reduces the number of passengers and thus the payload carried by the aircraft. It is worth noting that the Pareto front is not very smooth. This could have resulted from the step size being too large when exploring designs near the Pareto front. Alternatively, the unfeasible regions defined by the CG location and the in-ability to reach steady-state cruise are likely to have resulted in a very fragmented design space.

Due to the small population of the second Pareto front Fig. 14 does not show as clear of a trade-off as that in Fig. 13. Note that some of the designs in Fig. 14 lie at a significant distance from the second Pareto front. These designs have a high Φ_{H_2} and hence appear to be good in the first layer due to their small emissions, but are not necessarily optimal otherwise. This means that care must be taken in choosing design points, regardless of their performance lying on the first Pareto front. The capabilities of MDR are displayed by its ability to automatically discard such designs by the use of the nested dominance relations.

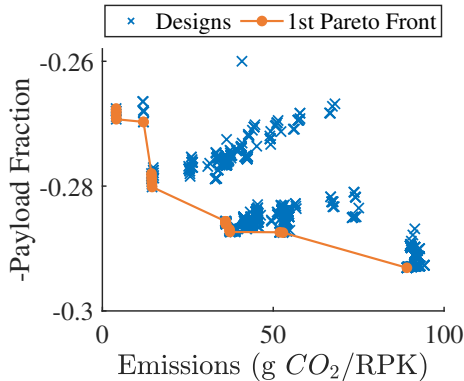


Fig. 13 First-layer performance distribution and Pareto front of the main optimisation run for current needs. Data obtained from aircraft flying the standard mission.

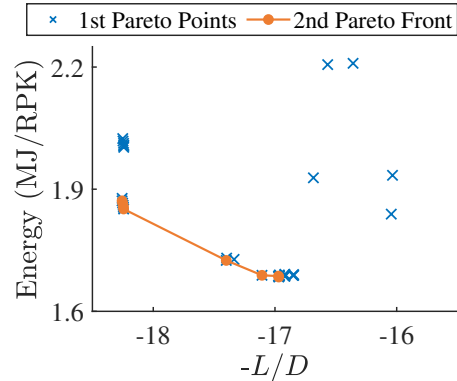


Fig. 14 Second-layer performance distribution and Pareto front of the main optimisation run for current needs. Data obtained from aircraft flying the standard mission.

2. Hybrid Optimisation for Future Needs

In the optimization for future needs, the performance distribution of the first layer is similar to that for the optimization for current needs (Figs. 13 and 15 respectively). This is expected because they use the same metrics for the first dominance relation. Some differences can also be observed. Fig. 13 displays fewer but more dispersed design clutters, whereas Fig. 15 shows a larger number of more concentrated design clutters. Figure 17 shows a direct comparison between both first-layer Pareto fronts for the current and future needs runs. As expected, the future needs run, which has a higher emphasis on emissions, is mostly able to obtain a Pareto front with lower emissions. This illustrates that changing the second dominance layer has a significant effect on the behaviour of the optimizer, irrespective of whether the metrics chosen for the first dominance layer are the same or not.

Figure 16 shows that the Pareto front of the performance distribution of the second layer is sparsely populated in the region with non-zero emissions. Nevertheless, it begins to reveal a trade-off between the energy and emissions per RPK.

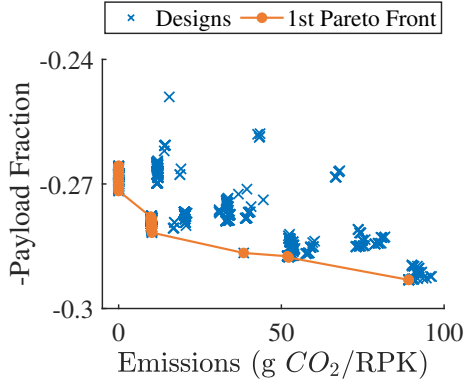


Fig. 15 First-layer performance distribution and Pareto front of the hybrid optimisation run for future needs. Data obtained from aircraft flying the standard mission.

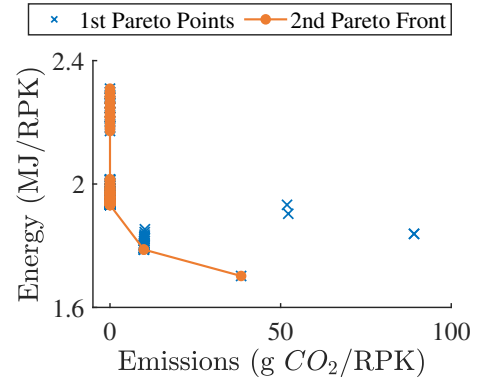


Fig. 16 Second-layer performance distribution and Pareto front of the hybrid optimisation run for future needs. Data obtained from aircraft flying the standard mission.

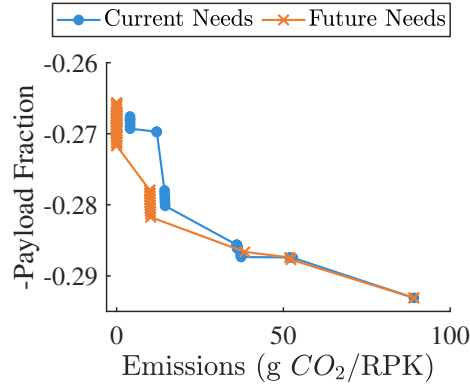


Fig. 17 Comparison of the first-layer Pareto front of both hybrid optimisation runs for current (blue) and future (orange) needs. The data was obtained from aircraft flying the standard mission.

C. Kerosene-Only Optimization

To identify the effect of the operating point on the overall aircraft performance, the first and second performance layers of the kerosene optimisation run have been provided in Figs. 18 and 19, and a comparison between the first-layer Pareto fronts of the hybrid and kerosene optimisation runs has been provided in Fig. 20.

Figure 18 reveals that the performance distribution for the kerosene-only run is more concentrated than for the hybrid optimisation run for present needs (Fig. 13). This is expected since the effect of changing Φ_{H_2} is very pronounced on

the emissions, justifying the lack of different clusters when Φ_{H_2} is zero. It can also be seen that most of the hybrid Pareto front is Pareto equivalent to the kerosene Pareto front. Analysis of the design space reveals that this is reasonable.

The kerosene optimisation run had one fewer dimension to explore than the hybrid run for the same number of allowed objective function evaluations. This means that the kerosene run is able to explore a greater proportion of its design space, resulting in a Pareto front with a higher resolution. This is validated by the fact that the kerosene run reached the minimum step size, whereas the other runs did not. Further support to this argument is given by the fact that the performance distribution of the second layer for the kerosene run (Fig. 19) has a larger spread than those for the hybrid runs (Figs. 14 and 16). Given that the kerosene-only design space is a subset of the hybrid design space, the Pareto front obtained from the kerosene run is more likely to be closer to the true overall Pareto front due to the significant advantage in payload fraction in kerosene-only designs, which results from the removal of the hydrogen tank.

Comparing the data from the kerosene optimized design and the ATR 72 (Table 1) reveals that the non-hydrogen factors have a maximum contribution to the reduction in emissions of about 9% for a range of 750 km. This reduction in emissions originates from flying with a more powerful engine than the ATR 72. As expected, similar trends can be seen in the present hybrid optimized design.

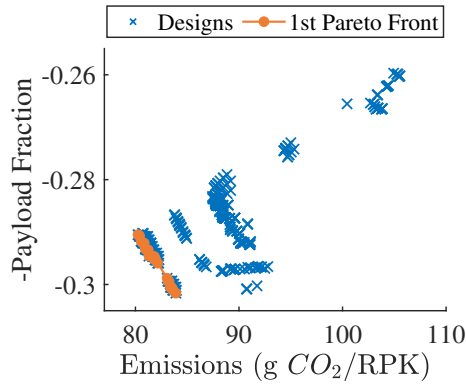


Fig. 18 First-layer performance distribution and Pareto front of the kerosene optimisation run for current needs. Data obtained from aircraft flying the standard mission.

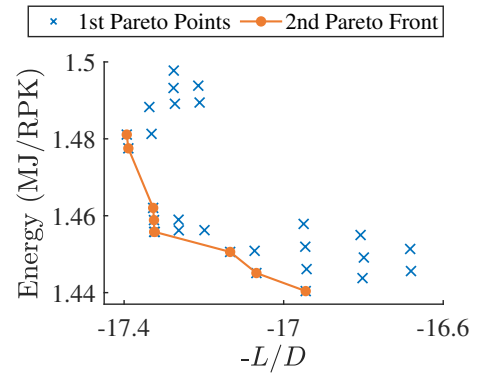


Fig. 19 Second-layer performance distribution and Pareto front of the kerosene optimisation run for current needs. Data obtained from aircraft flying the standard mission.

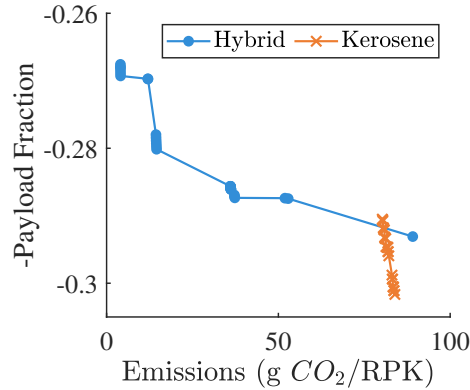


Fig. 20 Comparison of the first-layer Pareto front of both hybrid (blue) and kerosene (orange) optimisation runs for current needs. The data was obtained from aircraft flying the standard mission.

D. Characteristics of the Optimized Designs

The performances of the optimized designs have been plotted alongside the performances of a straight retrofit in Figs. 21 and 22. In Fig. 21 it can be seen that most of the optimized designs produce fewer emissions than the equivalent

straight retrofit. There are exceptions to this, which can be justified by the fact that the 1st layer optimized designs are the designs in the trade-off between emissions and payload fraction, and not just designs which minimize emissions. The benefit in emissions decreases with increasing Φ_{H_2} . This confirms the prediction earlier, which implies that the potential improvements in emissions per RPK decrease with Φ_{H_2} . This is a fundamental behaviour of all hydrogen hybrid aircraft since the emissions must be zero when $\Phi_{H_2} = 1$. This, however, does not mean that retrofits are as good as bespoke hydrogen designs. The primary setback of using a retrofit can be understood by studying Fig. 22.

As discussed in Section IV.A, the increase in energy per RPK with Φ_{H_2} is attributed to the space the hydrogen tank takes up in the cabin. This is a limitation that only retrofits have due to their limited cabin space. If a bespoke hydrogen aircraft design were to be made, the trade-off between the tank size and the number of passengers would not be as pronounced, allowing for even better performances than the current ones.

Nevertheless, for the optimization for current needs, most designs in the first Pareto front have significantly reduced energies per RPK relative to the straight retrofit (Fig. 22). The exceptions are again attributed to the trade-off present in the second dominance layer. Optimising for both emissions and energy per RPK has resulted in the current hybrid optimized design containing a modest amount of hydrogen (62%, Table 1). This low amount of hydrogen is critical to paving the way to full decarbonisation via on-the-go certification.

For the optimization for future needs, the increased importance of the emissions can be seen from the increased number of designs at $\Phi_{H_2} = 1$, which have zero emissions in Fig. 23. Most designs in the first Pareto front also have significantly reduced energies per RPK relative to the straight retrofit (Fig. 24). With more importance given to the emissions, some designs in the second Pareto front require more energy than the baseline. Optimising with an increased emphasis per RPK, and choosing the design with minimum emissions and energy requirements, has resulted in a design fully reliant on hydrogen (Table 1).

Table 1 shows that the key improvement made over the ATR 72-500 is using a more powerful engine. Furthermore, the optimized designs with hydrogen also cruise at a slightly lower speed. The cruise altitude of the ATR 72 appears appropriate for the rest of the designs. Overall, both of hybrid optimisation runs can be considered a success. With this, a study of how the 2050 goal to decarbonise aviation will be achieved can be made.

Figure 25 shows a potential path to the full decarbonisation of turboprop aircraft. It is clear that the kerosene optimized design can be implemented the soonest since it primarily requires only different engines, similar to the A320 NEO compared with the base A320. This similarity was used to estimate the kerosene hybrid development time as six years, which is the difference between the announcement of the A320 NEO [45] and its introduction to service [46]. Since carrying any amount of hydrogen will require a baseline amount of certification and another engine development, a further twelve years have been given for the development of the current hybrid optimized design. While speculative, this suggests a route by which the emissions from aviation might advance towards zero in the UK by 2050, the aim set by the Jet Zero Council [2]. Regarding the energy per RPK, although the decrease in energy required is lost as Φ_{H_2} is increased, the mission energy does not increase by a significant amount relative to the levels today.

Table 1 Characteristic data of the optimized aircraft and the ATR 72 model. The emissions (W_{CO_2}) were obtained by flying the aircraft at the standard mission. The input data for the ATR 72 was obtained from [43].

Quantity	Units	ATR 72 -500	Kerosene Opt. Design	Current Hybrid Opt. Design	Future Hybrid Opt. Design
Φ_{H_2}	%	0	0	62	100
n_{seats}	seats	68	68	56	48
$P_{eng, max.}$	kW	2050	3425	3490	3400
s	km	1 430	750	750	750
M	—	0.44	0.40	0.40	0.40
h	ft	17 000	15 900	15 900	17 500
W_{CO_2}	$g CO_2/RPK$	88	80	36	0

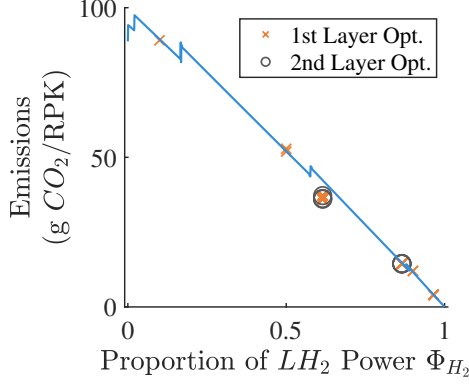


Fig. 21 Comparison between the emissions produced by a straight retrofit (blue line) and the hybrid optimized aircraft for current needs. In both cases the aircraft fly the standard mission.

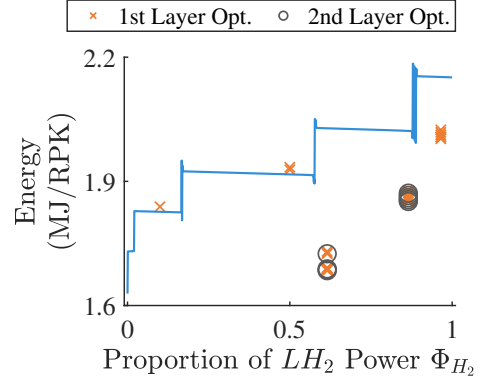


Fig. 22 Comparison between the mission energy of a straight retrofit (blue line) and the hybrid optimized aircraft for current needs. In both cases the aircraft fly the standard mission.

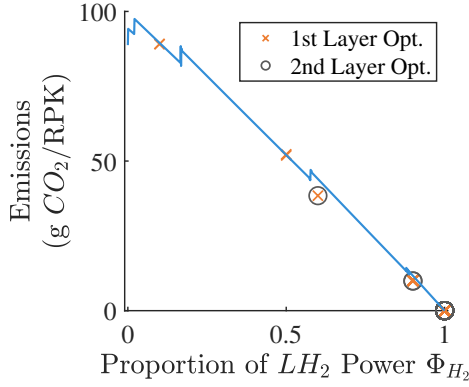


Fig. 23 Comparison between the emissions produced by a straight retrofit (blue line) and the hybrid optimized aircraft for future needs. In both cases the aircraft fly the standard mission.

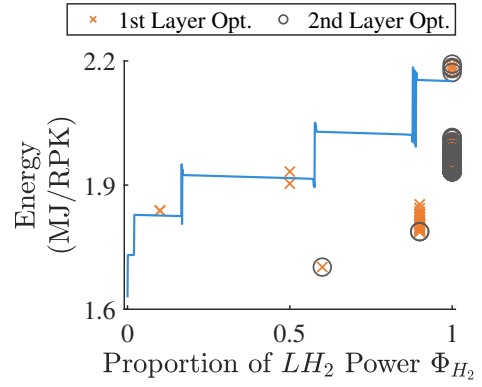


Fig. 24 Comparison between the mission energy of a straight retrofit (blue line) and the hybrid optimized aircraft for future needs. In both cases the aircraft fly the standard mission.

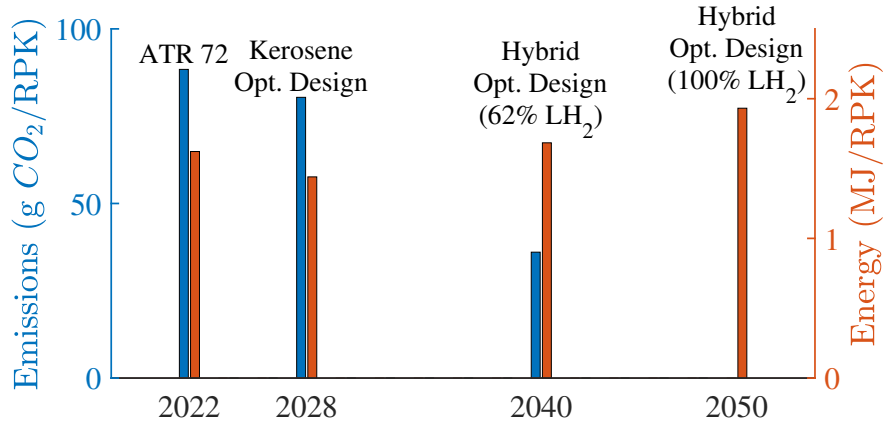


Fig. 25 Image representing a possible progression of aircraft leading up to 2050. Except for the ATR 72, the other aircraft are results of the optimisation performed in this investigation. The data was obtained from aircraft flying the standard mission.

E. Validation of the Aircraft Model and its Limitations

The emissions predicted by the model for a 750 km flight of the ATR 72 (88 g of CO_2 RPK) are similar to other models (79 g of CO_2 RPK) [41]. This corresponds to a difference of under 12%, hence validating the model to a first order. Further, the non-hydrogen emission improvements (attributed to the kerosene optimized design in Table 1) are of 9%. The kerosene optimized design has an engine with 40% higher maximum power, which requires this engine to be of larger size according to Fig. 7. Achieving reduced emissions with larger engines is expected, and hence has served as a first-order check for the optimiser.

It has been assumed in the Breguet range equation that the propulsive efficiency is constant regardless of the operating point, taking a value of 0.8. This is a representative value for modern aircraft, as stated in Raymer [34]. Nevertheless, X-Plane 11 performs its own aerodynamic simulation, meaning that this did not affect anything other than the calculated fuel mass required.

A decision was made to put the hydrogen tank in the middle of the passenger cabin, with its CG matching that of the empty aircraft. This was done in order to simplify the weight and balance calculations, but it significantly complicates the operation of the aircraft — half of the passengers would likely not even have access to a toilet in-flight. Given the small hydrogen tank size of the two hybrid optimized designs, the location of the hydrogen tank is less critical than was initially expected. It is therefore argued that the internal layout of the aircraft can likely be rearranged so that the needs of each operator are accommodated whilst also maintaining the aircraft CG within acceptable bounds. Even if the internal structure could not be rearranged in an acceptable way, it is worth noting that both the front and rear cabins would be able to evacuate since the emergency exits of the ATR 72 are not where the tanks would go.

The take-off model does not allow for take-offs at different power settings. This is important because the optimizer explores areas of the design space in which the maximum engine power is beneath that used for the take-off model. Secondly, no indirect emissions and energy requirements or equivalent warming effects were considered. Together, these shortcomings mean that the model can be further improved.

V. Conclusion

In conclusion, this study has been successful so far in able to help create understanding of the hydrogen combustion design space and provide a potential pathway to the decarbonisation of turboprop aircraft.

The chosen optimiser naturally generates Pareto fronts that approximate the fundamental trade-offs involved in hydrogen aircraft design. With this, the goal of bringing understanding to the hydrogen aircraft design space has been met. This study also revealed the need for a bespoke hydrogen aircraft design. This could be seen from the fact that the mission energy of the Pareto-optimal hybrid designs remains approximately constant. Since hydrogen is bound to be a more expensive fuel than kerosene currently is, further improvements in the energy per RPK are needed for air travel to still be as accessible. With this, the second goal to estimate the performance of hydrogen aircraft has been met.

A kerosene-only optimized aircraft was simulated in order to be able to quantify the effects of the non-hydrogen variables on aircraft performance. It was concluded that these factors allow for a maximum CO_2 emissions reduction of about 9% relative to the base ATR 72 flying the same route. A hybrid aircraft was subsequently obtained from an optimisation run that prioritised reducing both cost and emissions, reflecting current market needs. Considering these needs is especially important in the present day since hydrogen technologies are not yet mature and are therefore expensive. The aircraft obtained with the current market in mind is a hybrid design whose CO_2 emissions were 58% lower than those of the ATR 72, which is 49% better than the kerosene optimized design relative to the ATR 72. Finally, assuming that the cost of hydrogen-related technologies will decrease as technologies mature, a final hybrid run was performed with more relative emphasis on the CO_2 emissions. This resulted in a hybrid design that heavily relies on hydrogen and whose in-flight carbon emissions were negligible.

The above designs form the basis for a potential accelerated pathway towards the implementation of hydrogen technologies via on-the-go certification. This is because none of the hybrid designs relies completely on hydrogen, making it possible for them to operate safely with the remaining proportion of kerosene in case of an emergency. With this, it can be said that the third goal of the study has been met.

Having achieved all of the study goals to a satisfactory extent, this investigation has provided both validation to the design methods used and understanding of the hydrogen combustion design space. This small-scale exercise has now opened up the doors to larger-scale problems involving more parts of the whole system. It is the solutions to such problems that have the potential to be the catalysts for true change within the aviation industry.

Appendix

Consider the equation for the Brake-Specific Fuel Consumption (BSFC):

$$BSFC = \frac{\dot{m}_{fuel}}{P} \quad (14)$$

Where P is the engine power output, as given by the following equation:

$$P = \dot{m}_{fuel} \cdot C_{fuel} \cdot \eta_{th} \quad (15)$$

Where C_{fuel} is the specific energy of the fuel and η_{th} is the turbo-engine thermal efficiency. It is important to note that η_{th} is assumed to be independent of the fuel type in this derivation.

Now consider the fact that the turboprop engine combusts both hydrogen and kerosene simultaneously. Eq. (14) becomes:

$$BSFC = \frac{\dot{m}_{H_2} + \dot{m}_{JAI}}{P_{H_2} + P_{JAI}} \quad (16)$$

Substituting Eq. (15) into Eq. (16), and assuming that η_{th} is the same for both fuels, a new expression for the BSFC can be obtained:

$$BSFC = \frac{1}{\eta_{th} \cdot (P_{H_2} + P_{JAI})} \cdot \left(\frac{P_{H_2}}{C_{H_2}} + \frac{P_{JAI}}{C_{JAI}} \right) \quad (17)$$

The parameter that defines the ratio of power provided by hydrogen to that provided by kerosene can now be defined:

$$\Phi_{H_2} = \frac{P_{H_2}}{P_{H_2} + P_{JAI}} \quad (18)$$

This definition can be used in Eq. (17) to give a new expression for the BSFC:

$$BSFC = \frac{1}{\eta_{th}} \cdot \left[\frac{1}{C_{H_2}} \cdot \Phi_{H_2} + \frac{1}{C_{JAI}} \cdot (1 - \Phi_{H_2}) \right] \quad (5)$$

Now, using Eqs. (15) and (18), as well as the fact that $\dot{m}_{fuel} = W_{fuel}/T$ (where T is time), a relationship between the fuel masses, the specific energies of the fuels and Φ_{H_2} can be obtained:

$$\Phi_{H_2} = \frac{W_{H_2} \cdot C_{H_2}}{W_{H_2} \cdot C_{H_2} + W_{JAI} \cdot C_{JAI}} = \left(1 + \frac{W_{JAI} \cdot C_{JAI}}{W_{H_2} \cdot C_{H_2}} \right)^{-1} \quad (19)$$

This leads to the following expression for the ratio of masses:

$$\frac{W_{JAI}}{W_{H_2}} = \frac{C_{H_2}}{C_{JAI}} \cdot \left(\frac{1}{\Phi_{H_2}} - 1 \right) \quad (20)$$

The methods outlined in Section III.D provide a value for the total amount of fuel on board:

$$W_{fuel, net} = W_{H_2} + W_{JAI} \quad (21)$$

Using Eqs. (20) and (21), the mass of hydrogen can be found:

$$W_{H_2} = W_{fuel, net} \cdot \left[1 + \frac{C_{H_2}}{C_{JAI}} \cdot \left(\frac{1}{\Phi_{H_2}} - 1 \right) \right]^{-1} \quad (22)$$

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