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Optimal aircraft fleet and energy mix under limited availability of resources

Minimizing cumulative emissions under different scenarios for air traffic demand, energy resources and technological improvements.

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ABSTRACT

The substitution of fossil kerosene by alternative energy carriers is a prominent mitigation lever of the climatic impact of aviation. Yet, prospective aviation scenarios are subject to significant uncertainties concerning the future evolution of air travel demand, aircraft technology, and the availability of energy resources. A demand model was calibrated with socioeconomic data from the World Bank and used prospectively with data from the Shared Socioeconomic Pathways database. The Generic Airplane Model was used to design a set of aircraft with conventional and alternative propulsion systems, under varying technology scenarios. Then, optimal mitigation scenarios were generated using a Multidisciplinary Optimization methodology, by minimizing the cumulative carbon emissions of the sector with respect to the energy mix and the penetration of new aircraft on the current fleet. The scenario database also provided the production of biomass and electricity, which constrained the sectoral consumption of these resources, and for the carbon intensity of electricity production, which allowed to estimate emission intensity associated to electricity-based energy carriers. Finally, the implementation of scenario optimization is discussed, where the use of Differential Programming libraries allowed simultaneously for reducing implementation costs associated with these problems and a 65 to 78 speedup.

Keywords: Multidisciplinary Design Optimization; Aircraft Design; Shared Socioeconomic Pathways; Climate and Aviation; Alternative fuels;

NOMENCLATURE

AD	Automatic Differentiation
ASK	Available Seat-Kilometres
GAM	Generic Airplane Model
GDP	Gross Domestic Product
IAM	Integrated Assessment Model
MDO	Multidisciplinary Optimization
RCB	Remaining Carbon Budget

RCP Representative Concentration Pathways

RPK Revenue Passengers-Kilometres SSP Shared Socioeconomic Pathways

1.0 INTRODUCTION

From 1973 to 2018, aviation reduced by 79% fuel burn per revenue passenger-kilometer (RPK) transported [1]. Yet the CO2 emissions of the sector increased by 176% in the same period, mainly due to the severe 1236% increase in air traffic that was possible due to reduced ticket prices (linked to efficiency and operational gains), population increase and economic development. To pursue climate mitigation, aircraft design may have to shift from efficiency pursuit alone.

There are several levers to reduce CO2 emissions: reduce traffic growth, improvement in aircraft and operational efficiency, fleet renewal, using alternative fuels/energy sources and even novel aircraft architectures [2]. The two latter being particularly complex as their mitigation potential and speed of deployment depend on both the vehicle performance (design dependent) and the energy system used to produce the fuel/energy (regional and temporal dependency).

The design of future aircraft is discussed, with conventional and alternative propulsion systems. Trend and optimistic scenarios are made of the evolution of aircraft design parameters, and the resulting energy efficiency of designs is compared with a preliminary airplane design tool [3]. Accounted propulsion architectures are thermal propulsion powered by kerosene and hydrogen, or electric propulsion powered by hydrogen fuel cells or batteries.

Yet, the limited availability of biomass and clean energy, and the use of energy intensive processes can limit the production amounts of alternative carriers. Realizing industry's roadmaps would require 9% of global renewable electricity and 30% of sustainably available biomass in 2050 [4].

In this paper, we propose to use data from Integrated Assessment Models (IAMs) to construct sectoral aviation scenarios in the form of optimization problems. The air traffic demand is estimated from socio-economic indicators, the cumulative CO2 emissions of the global fleet is minimized, and the availability of energy resources is used to constrain the deployment of alternative aircraft (flying with liquid hydrogen and battery as energy carriers) and the biofuel/electrofuel blend in conventional aircraft.

Finally, implementation details are discussed. The use of hardware-accelerated high performance computing libraries [5] was linked to a Multidisciplinary Optimization (MDO) framework [6], which allowed for significant performance gains for the simulation and optimization of scenarios.

1.1 Scenarios as optimization problems

Decision-making can be formalized into prospective scenarios by using an optimization approach. Where scenario exploration is made automatically with optimization algorithms, but first the formalization of the optimization problem must be made by choosing the set of:

- Optimization variables: represent what parameters the optimizer may vary to find the optimal scenario.
- Constraints: expressed as a set of equality and inequality conditions, they represent the criteria used to define which scenarios are feasible.
- Objective function: the criteria to be maximized or minimized by the optimizer, it represents the metric used to compare feasible scenarios.

Multidisciplinary Optimization (MDO) frameworks are mainly used for the optimal design of vehicles/products, but its theory and methods can also be applied to Integrated Assessment Modeling. This work contributes to this research direction with: models to link data from global scenarios to sector-specific assessments, and methods to reduce computational burden of scenario optimization.

2.0 GLOBAL SCENARIOS

Integrated assessment models (IAMs) are simplified representations of physical and social systems, focusing on the interaction between economy, society and the environment. They represent the coupled energy-economy-land-climate system to varying degrees and are the main tools used by IPCC's Working Group 3 [7].

Here, we use data from the Shared Socioeconomic Pathways (SSP) [8]. Each SSP is created from a storyline to represent a consistent underlying logic to the depth of socioeconomic changes that societies are expected to have. These storylines are then used along with IAMs to quantify the baseline demographic and economic drivers. Energy service and final energy demand are then estimated from the resulting socioeconomic drivers, and the energy supply is computed from final to secondary to primary energies.

From each baseline scenario, mitigation scenarios are formulated by incorporating varying strategies concerning demand modification, renewable energy deployment and carbon sequestration strategies. Mitigation scenarios are named according to a target radiative forcing by the end of the century, these are made to match scenario emissions to Representative Concentration Pathways (RCP), which are used in the analysis carried by the IPCC Working Groups 1 and 2.

Figure 1 presents the socioeconomic drivers over baseline and the lowest emitting mitigation scenario for each of the SSPs. Some mitigation scenarios incorporate the effect of mitigation policies on socioeconomic drivers such as SSP2, 3 and 5. Figure 2 presents the energy system production in some baseline and intermediate mitigation scenarios.

2.1 Shared Socioeconomic Pathways (SSPs)

• SSP1: Sustainability – Taking the Green Road (Low challenges to mitigation and adaptation):

"The world shifts gradually, but pervasively, toward a more sustainable path, emphasizing more inclusive development that respects perceived environmental boundaries. Driven by an increasing commitment to achieving development goals, inequality is reduced both across and within countries. Consumption is oriented toward low material growth and lower resource and energy intensity" [9]. A particular focus is given to the diverging nature of policies in SSP1 relative to other SSPs, where mitigation is achieved by reducing final energy demand rather than increasing clean energy production (Figure 2).

• SSP2: Middle of the Road (Medium challenges to mitigation and adaptation):

"The world follows a path in which social, economic, and technological trends do not shift markedly from historical patterns. Development and income growth proceeds unevenly, with some countries making relatively good progress while others fall short of expectations. Global and national institutions work toward but make slow progress in achieving sustainable development goals" [10].

• SSP3: Regional Rivalry – A Rocky Road (High challenges to mitigation and adaptation):

"A resurgent nationalism, concerns about competitiveness and security, and regional conflicts push countries to increasingly focus on domestic or, at most, regional issues. Policies shift over time to become increasingly oriented toward national and regional security issues. Economic development is slow, consumption is material-intensive, and inequalities persist or worsen over time. Population growth is low in industrialized and high in developing countries" [11].

 SSP4 Inequality – A Road Divided (Low challenges to mitigation, high challenges to adaptation):

"Over time, a gap widens between an internationally-connected society that contributes to knowledge- and capital-intensive sectors of the global economy, and a fragmented collection of lower-income, poorly educated societies that work in a labor-intensive, low-tech economy. Technology development is high in the high-tech economy and sectors. The globally connected energy sector diversifies, with investments in both carbon-intensive fuels like coal and unconventional oil, but also low-carbon energy sources. Environmental policies focus on local issues around middle and high-income areas" [12].

• SSP5 Fossil-fueled Development – Taking the Highway (High challenges to mitigation, low challenges to adaptation):

"This world places increasing faith in competitive markets, innovation and participatory societies to produce rapid technological progress and development of human capital as the path to sustainable development. Global markets are increasingly integrated. There are also strong investments in health, education, and institutions to enhance human and social capital. At the same time, the push for economic and social development is coupled with the exploitation of abundant fossil fuel resources and the adoption of resource and energy-intensive lifestyles around the world" [13].

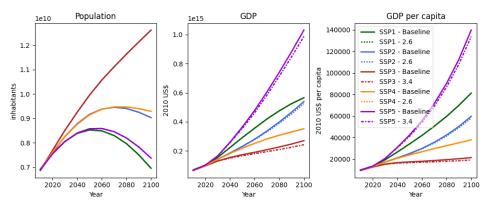


Figure 1: Socio-economic drivers in each SSP baseline and lowest-emitting mitigation scenario.

Data from [8].

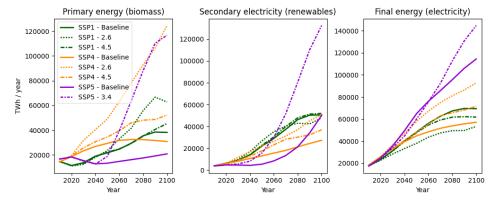


Figure 2: Biomass, renewable electricity and final electricity production in some SSP baseline and mitigation scenarios. Data from [8].

2.2 Estimation of air travel demand

There are several macroeconomic drivers to growth in air travel demand: disposable income, population growth, trade volumes, fuel prices, urbanization. In this work the effects of population and income are explicitly accounted for. In Equation 1, total demand is modelled as a per capita demand, influenced by per capita income, which is then scaled by the total population. World Bank data [14] supplied for historic Population and GDP and ICAO data [15] supplied for RPK historic data.

$$RPK = Pop \cdot RPK_{PC}$$
; $RPK_{PC} = f(GDP_{PC} = GDP / Pop)$... (1)

$$f(x) = L + (R - L) \left(\frac{C}{C + e^{-B(x - X)}}\right)^{1/\nu}$$
 ... (2)

Recent literature suggests the use logistic functions to estimate per capita transport demand as a function of per capita income [16]. Generalised logistic functions were used, due to their flexibility to be parameterized into logistic, sigmoid and Gompertz curves. Equation 2 presents the logistic curve, in which L is the left asymptote, R is the right asymptote, R is the position of the inflection point, and R is the logistic growth rate. R and R are extra parameters for greater flexibility, the first controls the duration of the transition from left to right asymptote, the latter controls near which asymptote maximum growth occurs.

The coefficients were calibrated to minimize the 2-norm of the error, resulting in a final ratio of the normed error to normed data of 10.6%. This yields an R2 of 0.954 and 0.967 respectively over the per capita data and the aggregated data, which was considered sufficient for the global prospective analysis carried.

The calibrated function was used to estimate the 2024 to 2050 RPK demand from GDP and Population data for each baseline scenario (Figure 3). COVID years were excluded from the calibration data, and its after-effects were considered by assuming that by 2024 per capita traffic will reach 2019 levels, this is achieved shifting the parameter X by the gap in income per capita between 2024 and 2019.

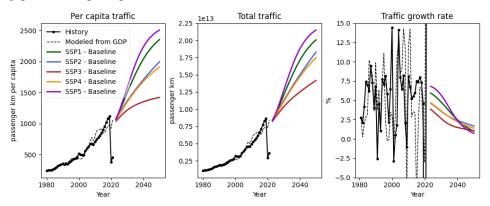


Figure 3: Baseline scenarios of per capita RPK, global RPK and RPK growth rate. Historical data from [14], [15].

3.0 PROSPECTIVE AIRCRAFT DESIGN

Several key energy carriers have emerged as potential substitutes of conventional kerosene. Recent literature lists synthetic kerosene (from bio-jet or power-to-liquid pathways), liquid hydrogen, ammonia, liquid natural gas, ethanol, methanol, and batteries as potential energy carriers for aviation [17]. Among these, only synthetic kerosene can be used (up to a 50% mixing ratio with conventional kerosene) in today's fleet without aircraft modifications.

Also, because of the specificities that each carrier imposes on the design, e.g., cryogenic fuel tank, fuel cells, electric motors, the architectures that employ each of them will have

very different trade-offs. The Generic Airplane Model (GAM) [3] was used as a preliminary airplane design tool, as it has extension to non-conventional architectures. It uses regression of historical airplane data to estimate airframe and structural weight and adds the propulsion system mass depending on architecture. Covered propulsion systems in this study are thermal propulsion powered by kerosene, hydrogen, or electric propulsion powered by hydrogen fuel cells or batteries.

3.1 Evolution of aircraft technology

Aircraft technology is expected to evolve in the coming years, especially with regards to unconventional architectures, as these technologies are maturing rapidly. Conservative, mid-optimistic and optimistic technology scenarios were made for a set of aircraft parameters.

Table 1 presents the 2020, 2035, 2050 values for the conservative and optimistic scenarios, mid-optimistic was taken as the mean between them. Figure 4 shows the evolution of some of these parameters with a collection of data points for comparison. Sources include technology roadmaps from IATA [18] and ATI [19], [20], [21], [22], ICCT aircraft design studies [23], [24], NASA electric propulsion studies and technology aspiration [25], [26], [27], [28], and EASA type certificate data [29].

Table 1
Quantitative evolution of aircraft technology parameters

	Unit	2020	2035	2050	Sources
Battery Specific Energy	Wh/kg	200	300-450	600-1200	[18], [24], [26], [27], [28], [29]
E-motor Specific Power	kW/kg	2	10-15	20-28	[21], [25]
Electronics Specific Power	kW/kg	2	10-15	22-30	[21], [28]
Fuel cell Specific Power	kW/kg	1	2-5	5-10	[18], [22], [25]
Fuel cell Efficiency	%	50	55-62	60-75	[22]
LH2 tank Gravimetric Index	%	20	25-35	40-70	[18], [20], [23]
Structural weight reduction	%	0	10-22	20-40	[18], [19]

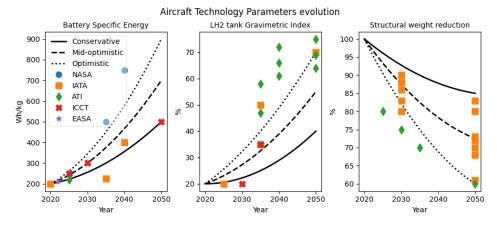


Figure 4: Evolution of aircraft parameters under conservative, mid-optimistic and optimistic technology scenarios.

3.2 Aircraft efficiency

For each propulsion system, an aircraft design is made with GAM, with varying missions:

- General aircraft: 6 passengers, 500 km
- Commuter aircraft: 19 passengers, 1500 km
- Regional aircraft: 120 passengers, 4500 km
- Short-medium aircraft: 250 passengers, 8000 km
- Long range aircraft: 550 passengers, 15000 km

Figure 5 shows the passenger efficiency, defined as the inverse of the specific energy consumption in MJ per travelled passenger-kilometer, of designs as a function of their year of entry-into-service. The 2019 reference from flights within the category range are also shown for comparison and are further presented in Table 2, obtained from the AeroSCOPE database [30].

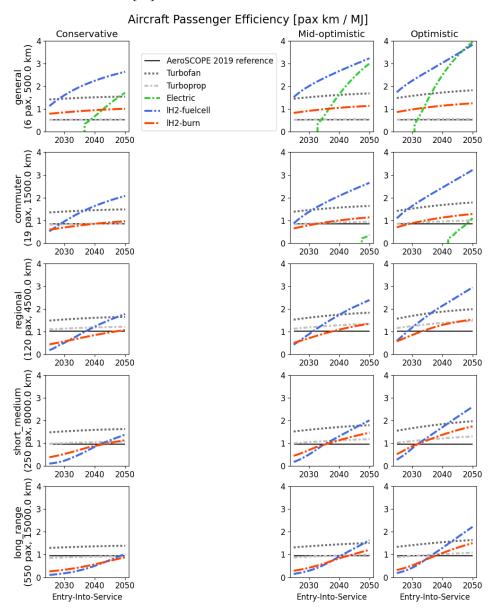


Figure 5: Passenger efficiency of prospective aircraft designs according to entry-into-service. Each row represents an aircraft category, each column a technology scenario.

4.0 OPTIMAL AVIATION SCENARIOS

There are several institutional and academic scenarios for the future of air transportation systems [2], [31]. Scenario outcomes can vary greatly according to assumptions used regarding evolution of demand [2], the carbon intensity of electricity [32] and the amount of aviation-available resources [4].

Aviation scenarios were generated from optimization problems, formulated to minimize the cumulative CO2 emissions of the sector by varying the penetration of new aircraft on the fleet and the energy mix of carrier production, subject to constraints on the annual consumption of energy resources (biomass and electricity).

4.1 Supply and demand

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Aviation scenarios were made to satisfy the RPK demand estimated from global SSP scenarios (section 2.2). Air traffic demand is expected to meet the scenario RPK. Available Seat-Kilometres (ASK) are calculated with a load factor that grows from 82.4% in 2019 to 85% in 2050 [33].

The choice of constraints and objective function have a direct impact on optimization results and must be made in line with the global scenario assumptions. For example, in the case of SSP1 the hypothesis that trend demand is reached is not in line with scenario storyline. In future research, low-demand scenarios could be made by constraining the cumulative CO2 emissions by a climatic target and choosing cumulative RPK as the objective to maximize, yielding scenarios that always respect targets and that limit the total demand based on resource availability.

4.2 Energy mix

Aviation's share of energy resources is set at 3.5%, which is the sector's 2019 share of final energy consumption [34]. The constraints on electricity and biomass consumption are defined as the aviation share of the total production under the chosen SSP scenario. A linear ramp is applied from 2025 to 2030, to represent the transition from a system that relies solely on fossil kerosene to one that can incorporate biomass and electricity as energy sources.

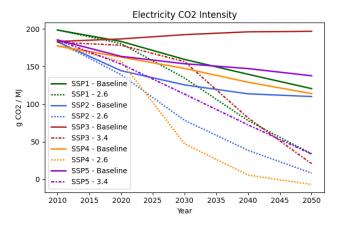


Figure 6: Carbon intensity of electricity in each SSP baseline and lowest-emitting mitigation scenario. Data from [8].

Regarding the aviation energy mix, a transitioning electricity grid is used (Figure 6). Gaseous hydrogen can be produced by electrolysis, gas and coal. Electrolysis efficiency grows from 66% in 2019 to 75% in 2050 [35]. Biofuels can be produced by Fischer-Tropsch (MSW and others), Alcohol-to-Jet, and HEFA (fog and others) pathways. Electrofuels can be produced from gas-hydrogen with efficiency of 45% in 2019 and 63% in 2050 [36]. The share of annual production that is allocated to each energy production pathway are called the energy mix variables.

4.3 Fleet composition

Traffic is divided into distance bands, which have a mean energy consumption and satisfy a fixed share of global demand. These shares correspond to the 2019 share of global ASK over all flights from the distance bands. The 2019 energy consumption and share of global ASK are extracted from the AeroSCOPE database [30] and are presented in Table 2.

It is assumed that all aircraft configurations can be introduced in any fleet segment, once introduced the share of supply covered by each aircraft follows a sigmoid function with limited growth rate up to a maximal aircraft share, which are the aircraft maximal penetration variables. The energy consumption of each aircraft is derived from section 3.2 with trend technology scenario and entry-into-service by 2035, except for the electric airplane with entry-into-service by 2040.

Table 2
Fleet categories and their maximum distance, share of ASK and energy consumption

Category	Max distance (km)	Share of 2019 ASK (%)	Mean 2019 energy consumption (MJ/pax km)
General	500	2.7	1.87
Commuter	1500	22.1	1.18
Regional	4500	38.6	0.97
Short-medium	8000	18.3	1.05
Long range	18000	18.3	1.13

4.4 Scenario outcomes

Results are presented for baseline and the lowest emitting mitigation scenario for each of the SSPs.

Figure 7 presents the ASK covered in each category and the aircraft decomposition over SSP4-2.6. This is the only scenario that features hydrogen aircraft in the short-medium category, which can be explained by the scenario's low carbon intensity of electricity (Figure 6) and the high final electricity production (Figure 2). In all optimized scenarios, no hydrogen aircraft is used in the long-range category, due to the fact that their lower passenger efficiency yields that hydrogen is best allocated for other categories.

Figure 8 presents the energy production and the decomposition into production pathways for SSP4-2.6. Overall the biomass consumption reaches the maximum allocated amount, preferably by pathways that are biomass-efficient with modest emission factors rather than low emitting ones that are not as efficient. Hydrogen is mainly produced by electrolysis, except in the near 2050 due to an increased competition for electricity.

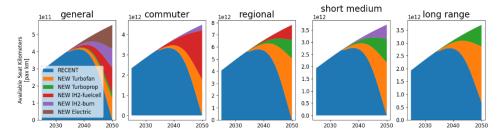


Figure 7: Category ASK and fleet decomposition into aircraft types for the SSP4-2.6.

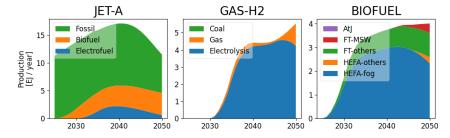


Figure 8: Energy production mix of carriers with multiple production pathways for the SSP4-2.6.

Figure 9 shows the consumption of energy resources, Figure 10 the carbon intensity associated to air travel supply and the total aviation emissions over selected scenarios.

Finally, Table 3 synthetizes the results for the simulated scenarios. The cumulative CO2 emissions are for the 2025-2050 period, which is also the objective function of the optimization problem. The Remaining Carbon Budget (RCB) used is for limiting warming to 2°C with 66% probability [37].

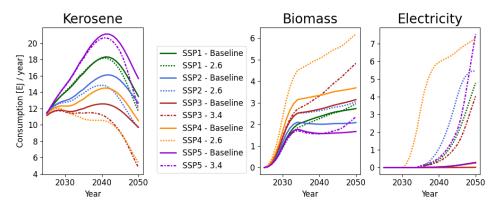


Figure 9: Consumption of energy resources in baseline and mitigation scenarios.

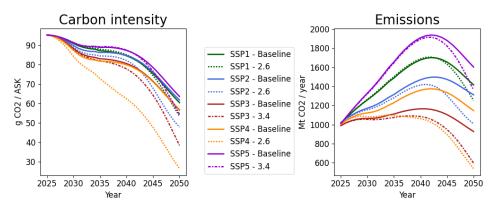


Figure 10: Carbon intensity of air traffic supply and total emissions from aviation in baseline and mitigation scenarios.

Table 3
Climate assessment in the context of Paris Agreement

Scenario	Cumulative CO2 emissions [Gt CO2]	Consumed share of RCB [%]
SSP1-Baseline	36.7	3.90
SSP1-2.6	36.4	3.87
SSP2-Baseline	33.1	3.53
SSP2-2.6	31.0	3.30
SSP3-Baseline	27.2	2.89
SSP3-3.4	25.0	2.66
SSP4-Baseline	30.8	3.27
SSP4-2.6	24.8	2.64
SSP5-Baseline	40.7	4.33
SSP5-3.4	39.8	4.23

5.0 IMPLEMENTATION

Scenarios are intrinsically time-dependent and may have many more variables than design models. Therefore, using them with optimization may come with implementation and simulation burdens.

First, the scenario must be executed several times in an optimization loop. Secondly, if there are many optimization variables derivative-free optimizers may scale badly and require the use of derivative-based algorithms. Traditionally, this leads to either using finite-differences (leading to longer execution times for many variables) or manually implementing derivatives (leading to extra implementation efforts).

In this work, the implementation and execution burdens were avoided by using Differential Programming libraries for modelling, which allowed for overall reduction of lines of code and accelerated execution.

5.1 Differentiable programming

Computer programs are a sequence of elementary commands (also referred to as computation graph) assembled with the intention to perform a task. Differential programming is a paradigm in which computer programs can be differentiated end-to-end automatically, [38] defines its purpose as "not merely the differentiation of programs, but also the thoughtful design of programs intended for differentiation".

There are many available libraries that allow for Automatic Differentiation (AD) of lines of code. Among these, JAX [5] was chosen because it encompasses configuration optimizations on CPU, GPU and TPU, and because its focus is on scientific computing in general, not just machine learning.

5.2 GEMSEO-JAX

JAX is a python library for high performance numerical computing. It has a similar interface to NumPy [39], but also features many extra transformations, such as: compilation of python code, vectorization over batches of data and AD.

GEMSEO is a python engine for multidisciplinary exploration and optimization [6]. GEMSEO-JAX [40] is a developed plug-in that allows for interfacing JAX models automatically into a GEMSEO process.

Many of the drawbacks of using IAMs for design can be addressed by using JAX. Execution times are reduced for system simulation (each iteration is faster) and for system optimization (gradient-based algorithms require fewer iterations). In future research, the vectorization over batches of data may also be used to handle uncertainty quantification and regionalization of scenarios.

5.3 Performance gains

For benchmarking performance, a reference scenario is made with only 3 categories, in order to compare with AeroMAPS [31].

Table 4
Benchmark over a single scenario execution

	Execution (s)	Linearization (s)
Original model	1.286	6.511
JAX version	0.256	0.009
Speedup	5.0	705.0

Over a single execution JAX performs 5 times faster than the original implementation. Over a linearization, the AD performs 705 times faster than finite-differences (Table 4). It is also important to note that JAX requires an extra compilation time of 2.291 seconds at the first execution, which was excluded from the single execution benchmark.

Table 5
Benchmark over an optimization loop

Algorithm	Derivative-based	Model	Iterations	Total time (s)
COBYLA	No	Original model	335	435.5
		JAX version	352	6.7
		Speedup	0.9	64.8
SLSQP	Yes	Original model	24	602.7
		JAX version	31	7.75
		Speedup	0.8	77.8

Over an optimization loop the JAX model performs around 65 and 78 times faster, respectively for derivative-free and derivative-based algorithms (Table 5).

6.0 CONCLUSION

Due to their heterogeneity, IAMs are difficult to compare and harmonize. We showcase the example of air travel demand, which often is not explicitly disaggregated from overall transport demand, requiring the calibration and extrapolation of new models to link IAM data to the variable of interest.

The performance of alternative propulsion systems is heavily dependent on the technological evolution of these novel systems, and relying on optimistic trends overestimates the suitability of non-conventional aircraft. When looking at the suitability of these new aircraft as climate mitigation policies, it is shown that vehicle performance plays a significant role, but the influence of the background energy system is also non-negligible, especially for aircraft with electricity-based energy carriers. With regards to biofuel incorporation, the constraint on annual biomass consumption significantly reduces the achievable mix with fossil fuels, crossing the 50% blend threshold would require priority access to biomass.

Results show that air traffic still grows in all scenarios, but with a decreasing growth rate due to the stabilization of personal propensity to travel as incomes grow. In most of the analyzed scenarios, aviation consumes more than 3% of the Remaining Carbon Budget for the $+2^{\circ}$ C target. The scenario features that allow for this limit not to be crossed are low air traffic demand and the introduction of low-emission aircraft, but only if there is an early availability of low-carbon electricity.

Implementation with JAX allowed for significative performance gains for optimizing scenarios, in the order of 65 to 78 times. These performance gains are important for using models for decision-making and are fundamental for addressing the shortcomings of using IAMs in MDO such as the temporal dimension, but also uncertainty quantification and regional disaggregation in future works. Also, the general use of JAX in MDO is shown to significantly reduce implementation and often lead to performance gains (especially for large models such as the one used).

Finally, because of the low fidelity of the models used and the uncertainty concerning future outcomes, working on validation is required before the use of obtained results as quantitative analyses.

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