

Sustainability meets AI: the potential of coupling advanced materials science with life cycle assessment towards industry commons [†]

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Abstract: The transformation of the aeronautical industry towards sustainable and cost-effective manufacturing is essential for enhancing aircraft performance, while reducing environmental impacts and production costs. This study integrates Life Cycle Assessment (LCA), Life Cycle Costing (LCC), and machine learning to enhance sustainable design in aeronautics. A Multi-disciplinary Optimization (MDO) approach was applied to a composite airframe panel, revealing that increased panel mass elevates Climate Change (CC) and Resource Use (fossils) impacts, largely due to carbon fiber and energy-intensive manufacturing. A Random Forest model predicted LCA/LCC outcomes, facilitating real-time, sustainability-driven decisions. Optimization reduced environmental impacts by 15%. Recommendations include bio-based composites and renewable energy use to further lower environmental costs.

Keywords: Life cycle assessment; life cycle cost; composite airframe parts; Machine learning

1. Introduction

The aeronautical industry faces a need for transformation, especially in the adoption of advanced composite materials. This shift is driven by the goals of enhancing aircraft performance, increasing productivity, and reducing manufacturing costs with more sustainable materials and innovative technologies. A transition to composite materials promises significant benefits, including cost savings, reduced weight, and lower fuel consumption, which together contribute to more efficient and environmentally friendly aircraft fabrication. Although thermoset polymer carbon fibre composites are widely used in the industry, recent trends indicate that thermoplastic composites are becoming popular due to their increased usage. Research indicates that employing thermoplastic composites resulted in a 10% reduction in weight in comparison to thermoset materials [1]. Thermoplastic composites are also excellent sustainable materials because they can be recycled and repaired, and they have short processing times.

One initiative addressing this need is the EC-funded project DOMMINIO, which seeks to integrate Life Cycle Assessment (LCA) and Life Cycle Costing (LCC) with artificial intelligence (AI) and multifunctional design variables for aircraft parts. DOMMINIO aims to support sustainable decision-making by linking design variables to sustainability indicators, providing an evidence-based approach to developing machine learning algorithms and predictive analytics for engineering applications. Specifically, the project's approach consists of: (i) conducting correlation studies between sustainability indicators and design variables to develop robust machine learning

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models, and (ii) utilizing predictive analytics to enable engineers and designers to make sustainability-oriented decisions throughout product development, as well as in maintenance, repair, overhaul (MRO), and end-of-life (EOL) management.

To illustrate the DOMMINIO framework in practice, a case study on a multifunctional composite stiffened airframe access panel is being conducted. This panel is assessed for environmental and cost implications across its life cycle. The panel consists of thermoplastic composite and thermoplastic filaments enhanced with nanoengineered materials, including magnetic nanoparticles for disassembly functionalities and continuous carbon nanotube fibers for heating and de-icing capabilities. Advanced manufacturing methods are employed in the panel's production: Automated Fiber Placement (AFP) is used to fabricate the panel, while Fused Filament Fabrication (FFF) is applied to print the gyroid stiffeners, reinforced with a top layer of AFP thermoplastic composite.

In sum, DOMMINIO seeks to set a new frame in sustainable aeronautical manufacturing by integrating advanced materials, nanoengineering, and AI-driven decision support. This holistic approach has the potential to redefine material selection and manufacturing processes in the aeronautical industry, supporting the dual goals of economic efficiency and environmental responsibility.

2. Methodologies

2.1. Life Cycle Analysis and Life Cycle Costing

Life cycle assessment is a standardized methodology by ISO14040/44:2006, widely applied to assess the potential environmental impacts of a product through the entire life cycle, from raw materials to manufacture, operation and end-of-life phase. An LCC study should include the cash flows for all life cycle stages (LCSs) starting from the planning and designing stage, continuing with the materials or components suppliers, product manufacturing, use stage and finally, the End-of-Life (EoL) stage [2].

For life cycle cost (LCC) methodology, the only standard that currently exists is the ISO 15686-5:2017, providing specifications and instructions for carrying out LCC analyses of building structures and their components.

In this study, the LCC is implemented in parallel with the LCA at the same system boundaries and its framework is based on the four LCA phases: i) goal and scope definition, ii) Life Cycle Inventory (LCI), iii) Life Cycle Cost Assessment (LCCA) and iv) interpretation of the results [3].

The goal of the life cycle environmental and cost assessment is to quantify the potential environmental and cost impacts of the initial design of multi-functional thermoplastic composite airframe parts developed in DOMMINIO project, to be used as alternative solution in conventional aircraft manufacture, and evaluate their sustainability towards recyclability, repairing and re-use.

2.2. Dynamic Life Cycle Analysis and Life Cycle Costing through Machine Learning

To convert Life Cycle Assessment (LCA) and Life Cycle Costing (LCC) from static to dynamic analyses, a machine learning (ML) toolkit was employed. The machine learning models were trained on simulations outputs to predict LCA and LCC outcomes under varying conditions. This dynamic approach enables continuous updates to predictions as new data becomes available, allowing the optimization framework to adapt in real-time. Consequently, environmental and cost impacts are more accurately represented throughout the design process, thus supporting sustainable decision-making.

2.2. Generation of Environmental and Cost Indicators

The LCA and LCC assessments were performed first on the initial design of the demonstrator part to produce a range of environmental and cost indicators essential for evaluating afterwards the sustainability and economic aspects of different design options. Initially, correlations between design parameters and LCA/LCC input parameters were identified, as detailed in Table 1. The output design parameters have been correlated to LCA input variables. The LCA study of the initial design, has revealed the key impact indicators that mainly include Climate Change (CC) and Resource Use of fossils (RUf), followed by Ionizing Radiation (IR), Acidification (AC), and Eutrophication (EF). These 5 impact indicators contribute at least 80% to the total single score. Concurrently, the design parameters have also been linked to LCC inputs and initial analysis produced indicators such as Cost of Materials (CoM), Cost of Utilities (CoU), and Cost of Waste (CoW) and Net Present Value (NPV).

LCA/LCC input parameters	Design parameters
Panel Input: the panel thickness as variable would correspond to different mass, manufacture energy, waste and total manufacture cost.	Panel thickness: The structural model would provide a panel of variable thickness.
Gyroids Input: stiffener dimensions would affect the material quantity (M2), manufacture energy, the amount of waste generated and total manufacture cost.	Stiffener dimensions: these are related to the occupied volume of the gyroids filling the stiffener.
cCNT filament: the total length of the cCNT filament as a variable will provide different mass, energy and cost input values.	SHM Sensor Network: the total length of sensor to meet probability of detection requirements
MNPs input: the area will correspond to TP resin with embedded magnetic nanoparticles different mass and cost input data.	Magnetic Nano-particle layers: the area of interface between stiffeners and panel
cCNT filament: the total length of the cCNT filament as a variable will provide different mass, energy and cost input values.	Heating elements: Total length around periphery of panel to meet de-icing requirements

Table 1: Correlation of design parameters and LCA/LCC input variables

The optimized dataset comprised three key panel components: composite bottom panel mass (M1), top composite reinforcement mass (M2) and the three stiffeners mass (M3). Each component has associated LCA and LCC indicators, creating a representative sample of the design configuration. This dataset captures the interdependencies between panel masses and their environmental and cost impacts, forming the foundation for predictive modeling.

2.3. Machine Learning Model Development and Training

To support decision-making, a machine learning model was developed and trained on this dataset to predict LCA and LCC identified key indicators based on input values for the three masses (M1, M2, M3). Utilizing machine learning in this context allows for rapid evaluation of environmental and cost impacts, reducing the need for repetitive, time-consuming recalculations and enabling efficient exploration of the design space.

For this project, the Random Forest algorithm was selected. This robust tree-based method is well-suited for moderate-sized datasets, which are common in specialized engineering applications. The algorithm's ability to handle a range of input features and resistance to overfitting make it ideal for predicting complex environmental and cost indicators based on varying design parameters.

Following standard machine learning practices, the data was divided into a training set to teach the model and a test set to validate its performance on unseen data. This

separation ensures the model's reliability and generalizability beyond the cases it was trained on.

2.4. Model Performance Evaluation

The performance of the Random Forest model was assessed using Mean Squared Error (MSE) and the Coefficient of Determination (R^2). MSE measures the average squared prediction error, with a lower MSE indicating higher accuracy. R^2 reflects how well the model's predictions correspond to actual data, with values closer to 1 indicating that the model effectively captures the variance in the output data.

The model demonstrated low MSE values and high R^2 scores on both the training and test sets, indicating excellent predictive accuracy and strong generalization to new data. These results suggest that the Random Forest model effectively learns the relationships between panel masses and LCA/LCC indicators without overfitting.

3. Model Integration with the Optimization Framework

To integrate the machine learning model with the optimization framework, the trained Random Forest model was serialized in joblib format, preserving its structure and parameters for consistent use without retraining. This serialized model significantly reduces computational demands and ensures efficient deployment within the optimization process.

Additionally, a Python script was developed to facilitate model interactions. This script searches for an input file, "input.csv," containing panel mass values (M1, M2, M3) generated by optimization procedure, formats the data for the model, and predicts environmental and cost indicators. These predictions are then saved in an output file, "output.csv," which includes indicators such as Climate Change, Resource Use, Ionising Radiation, Acidification, Eutrophication and Net Present Value.

For ease of use, the Python script was packaged as an executable, allowing it to run on any system without Python or additional dependencies. This streamlined setup provides stakeholders with a simple process to generate updated predictions by modifying the "input.csv" file, thus facilitating iterative design and optimization within the optimization framework that searches for various design solutions of the component under study.

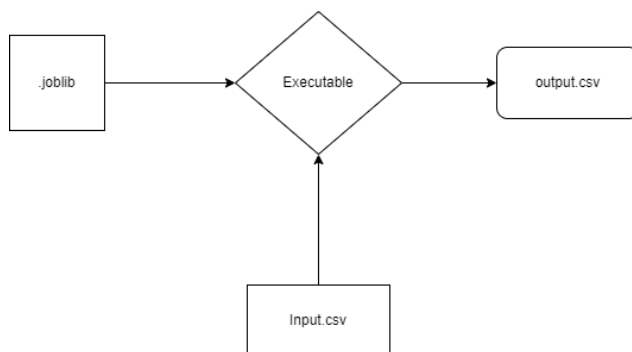


Figure 1: Visualization of executable flow of LCA/LCC module in Python script.

3. Results

3.1. Generation of Pareto-Optimal Data

In the case study, a comprehensive set of Pareto-optimal data was generated to represent three key masses in the prototype: panel (M1), top reinforcement (M2), and stiffeners (M3). This dataset was derived through a Multi-disciplinary Optimization (MDO) process that considered multiple objective functions and constraints to identify the best trade-offs among conflicting objectives, such as weight and strength. An analytical summary of the MDO data is presented in Table 2, providing key statistical insights, including mean, median, standard deviation, and range.

M3: Gyroid Mass	M2: Stiffener Mass	M1: Panel Mass	
614	614	614	Count
2.38	0.21	8.24	Mean
0.23	0.01	0.76	Std
1.83	0.16	6.63	Min
2.20	0.20	7.68	25%
2.38	0.222	8.08	50%
2.55	0.228	8.83	75%
2.91	0.23	9.61	Max

Table 2: MDO data description.

3.2. Life Cycle Impact Assessment (LCIA)

The LCIA focused on the manufacture phase based on the design optimisation data, with a specific emphasis on single score provided by the five key impact indicators: Climate Change (CC), Resource Use (fossils) (RUf), Acidification (AC), Eutrophication (EF), and Ionizing Radiation (IR). Key findings for each impact category are summarized as follows:

Climate Change (CC) and Resource Use (RUf): The LCA analysis for the studied case revealed that both indicators increase with higher panel mass (M1). At elevated panel mass values, the single score for CC is offset by a lower gyroids mass (M3), while variations in stiffener top reinforcement mass (M2) do not significantly affect these indicators. A similar pattern was observed in the RUf indicator, with higher panel mass correlating with higher single score. This is attributed to the high impact contribution of materials, mainly from the energy-intensive production of carbon fibre for panel mass (M1) and the high manufacture energy per kg output attributed to the FFF technology for fabricating the stiffeners at gyroid's structure (M3), deriving from fossil-based electricity.

Acidification (AC): Acidification was observed to increase primarily with the 3D printed stiffeners mass (M3). This rise is largely due to the energy-intensive 3D filament printing of the stiffeners 'gyroids' structure and the energy source mix of electricity.

Eutrophication impacts were more sensitive to increases in panel and top reinforcement masses (M1 and M2), while variations in gyroids mass (M3) had minimal influence. The eutrophication process, driven by excess nutrients, has significant adverse effects on aquatic ecosystems and, indirectly, on human health.

Ionizing Radiation (IR): Analysis of the (IR) indicator suggested that increased panel mass values have a considerable effect on this score. Even at low gyroid masses (M3), high panel mass values influenced IR scores significantly. Higher values of gyroids mass combined with lower panel mass also showed a notable effect, likely due to the energy requirements of these materials.

3.3. Life Cycle Cost Analysis (LCC)

The LCC analysis, linked to the MDO design optimization, examined all possible cost categories such as: Cost of Materials (CoM), Cost of Utilities (CoU), and Cost of Waste (CoW). Due to the fact that some costs occur in different periods, Life – Cycle Cost was expressed as the NPV (Net Present Value) of all costs. Findings include:

Cost of Materials (CoM): The cost of raw materials increased with higher panel (M1) and gyroids (M3) masses. The materials used, including thermoplastic composite tapes for AFP and polyether-ketone-ketone (PEKK) resin for FFF applications, were identified as particularly costly for aviation applications.

Cost of Utilities (CoU): Utility costs were observed to increase with larger quantities of gyroids mass (M3), highlighting the energy demands of this component's production.

Cost of Waste (CoW): Waste treatment costs followed a similar trend as material costs, with higher expenditures linked to the thermoplastic prepreg tape used in AFP manufacturing for the bottom panel and stiffeners' top reinforcement. Since FFF technology is regarded as a low-waste process, the waste costs are primarily due to AFP-related scrap.

Estimations on other cost categories such as Cost of Externalities (CoE), Cost of Depreciation (CoD) and Cost of operating Labour (CoL) had a minor impact or variation regarding mass.

3.4. Life Cycle Assessment (LCA) and Life Cycle Costing (LCC) Integration with MDO Data

The LCA/LCC analysis on the complete life cycle was developed into a module that integrates MDO optimization data, extending across the operational/use and end-of-life phases. Multifunctional elements embedded in the system were also incorporated. The resulting visual graphs illustrate the complete LCA (focusing on five impact indicators per life cycle stage) and the net LCC value post-MDO integration.

Climate Change Sensitivity to Mass Variables: The climate change single score was notably affected by the mass of both the bottom laminate and the gyroids (M3). The greater the UD tape mass in the bottom laminate, the higher the climate change score across the three life cycle stages.

Reduction of Environmental Impact through Optimization: During the LCA/LCC integration with MDO optimization, the climate change and resource use (fossils) indicators were highly sensitive to variations in bottom panel mass. The AFP bottom panel was identified as the primary environmental hotspot. As bottom laminate mass decreased, overall environmental impacts were reduced. Under optimized conditions, the single score of Climate Change ranges over 15% from the maximum to minimum value, while this range in the LCC-NPV is 1.3%.

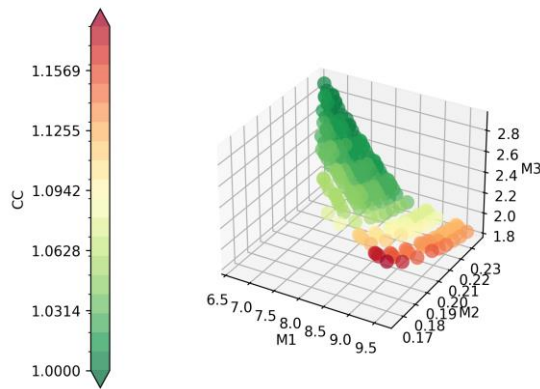


Figure 2: MDO design optimisation data and Single score of Climate Change (normalised)

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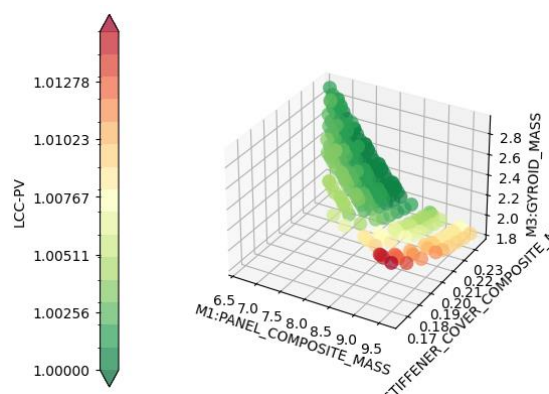


Figure 3: MDO design optimisation data and normalised LCC-Net Present Value

3.5. Future Recommendations for Environmental Impact Reduction

To further minimize environmental impacts, potential future approaches include increasing the bio-based content of composite materials and adopting renewable energy sources for electricity consumption in FFF technology. These recommendations could reduce fossil-based energy consumption and support long-term sustainability goals.

4. Conclusions

This study successfully integrated Life Cycle Assessment (LCA), Life Cycle Costing (LCC), and machine learning-driven Multi-disciplinary Optimization (MDO) to advance sustainable design in the aeronautical industry. An LCA and LCC analysis was first conducted for the initial design and then expanded across optimized mass configurations, providing insights into how different mass distributions impact environmental and cost indicators. A machine learning model, developed to predict these indicators, was packaged into an executable format, enabling streamlined application across varied design inputs. This approach reduced environmental impacts by 15%, showcasing the potential of integrating AI with lifecycle analyses. This framework holds promise for broader applications across the industry.

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