# Aircraft Paint System Optimization Workflow using a Combination of deterministic and data-driven Tools

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Abstract

The skin of a modern aircraft is composed of multiple layers of protective and decorative materials on top of carbon-fiber-reinforced plastic (CFRP) as the structural element of the fuselage and the wings (Fig. 1). As this paint system is characterized by a number of physical and structural properties (e.g. coefficient of thermal expansion, Young's modulus, Poisson ratio, layer thickness, etc.), finding an ***optimized*** paint system configuration which can withstand the environmental conditions it is exposed to during operation is a challenging task.
Among others, the strong variation in temperature, ranging from +45°C (on the ground) to -55°C (at cruising altitude) is one of the major factors that lead to stress within the materials. Deterministic approaches, e.g. finite element (FE) analysis and atomistic simulation (density functional theory, DFT, & molecular dynamics, MD) are efficient predictive tools for mechanical stress and materials properties, respectively. However, the identification of key properties for low thermal stress and materials with respective properties for an optimized paint system is challenging and time-consuming. Data-driven approaches, on the other hand, enable optimization by using large amounts of data and mapping of input (materials properties) and output (thermal stress) and inversely determine the optimal parameters. Unfortunately, the lack of suitable and extensive data sets often limits the use of ML.
In this work, the authors report recent results from their lab regarding utilizing machine learning (ML) in conjunction with FE, DFT and MD simulations to build an integrated tool stack for the efficient design of future aircraft paint systems (Fig. 2). For this purpose, the thermal stress of a state-of-the-art paint system is simulated using an FE model which takes into account relevant materials properties and allows the rapid generation of large amounts of data. The generated data set is then used for training and testing different ML models in order to identify the one with the best accuracy and hence highest representativity (surrogate model). Consecutively, the main drivers for thermal stress can be identified using correlational approaches and explainable artificial intelligence (AI) tools (SHapley Additive exPlanations) and optimized values for low thermal stress can be derived for the given paint stack in real-time.
Furthermore, a workflow for the prediction of polymer properties considering their chemical structure was implemented. Based on polymeric structures taken from databases, promising monomers have been selected and a conformation search using DFT and MD has been performed. The resulting electronic properties have been used to form polymer chains from the conformers with the lowest energy by employing the self-avoiding random walk procedure. After applying a force field and equilibrating the system the bulk properties of the formed polymers have been determined in order to identify promising materials that meet the optimized parameters of the above mentioned paint system. The simulation of polymers of interest allows the identification of materials with the desired properties while gaining a deeper understanding for the structure-property relationship of such materials. Furthermore, the generation of large amounts of simulation data based on polymers with different chemical structure enables an optimization process to rapidly predict polymer materials with optimized parameters.
The presented combination of deterministic simulation and data-driven modeling represents a tool set that allows an ***inverse design*** of aircraft paint systems, i.e. derive optimal paint system configurations for their specific applications and operating conditions, from the microscopic to the macroscopic scale in real-time and proves the power of such a workflow for the development of new materials and material systems without the need for large amounts of data. Next developments will consider adding paint aging models that have the potential to predict the in-service performance of such paint systems, thus predicting maintenance intervals or the entire life span of coatings until failure.

## References

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## Figures

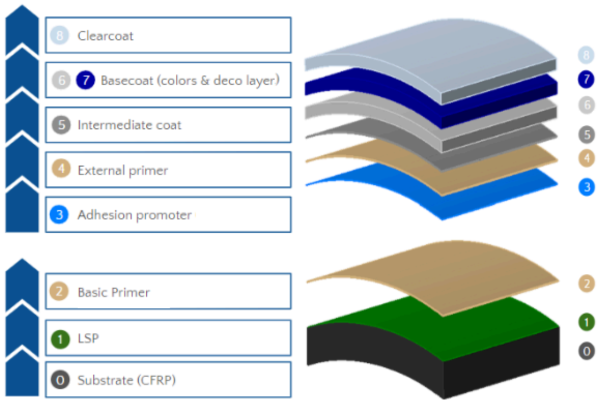


**Figure 1.** State-of-the-Art Paint System for Composites.

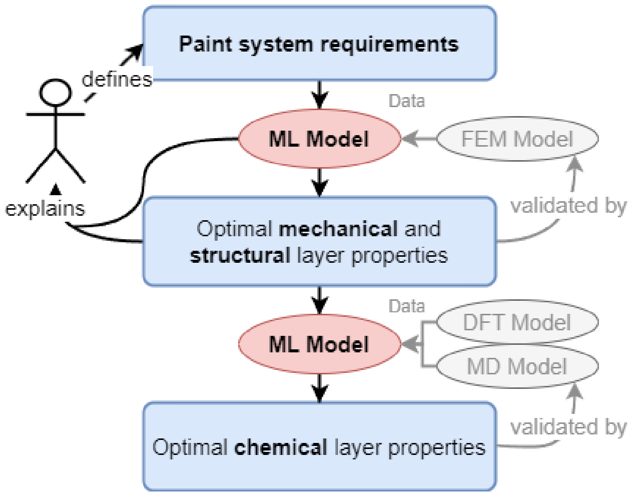


**Figure 2.** Paint System optimization Workflow.