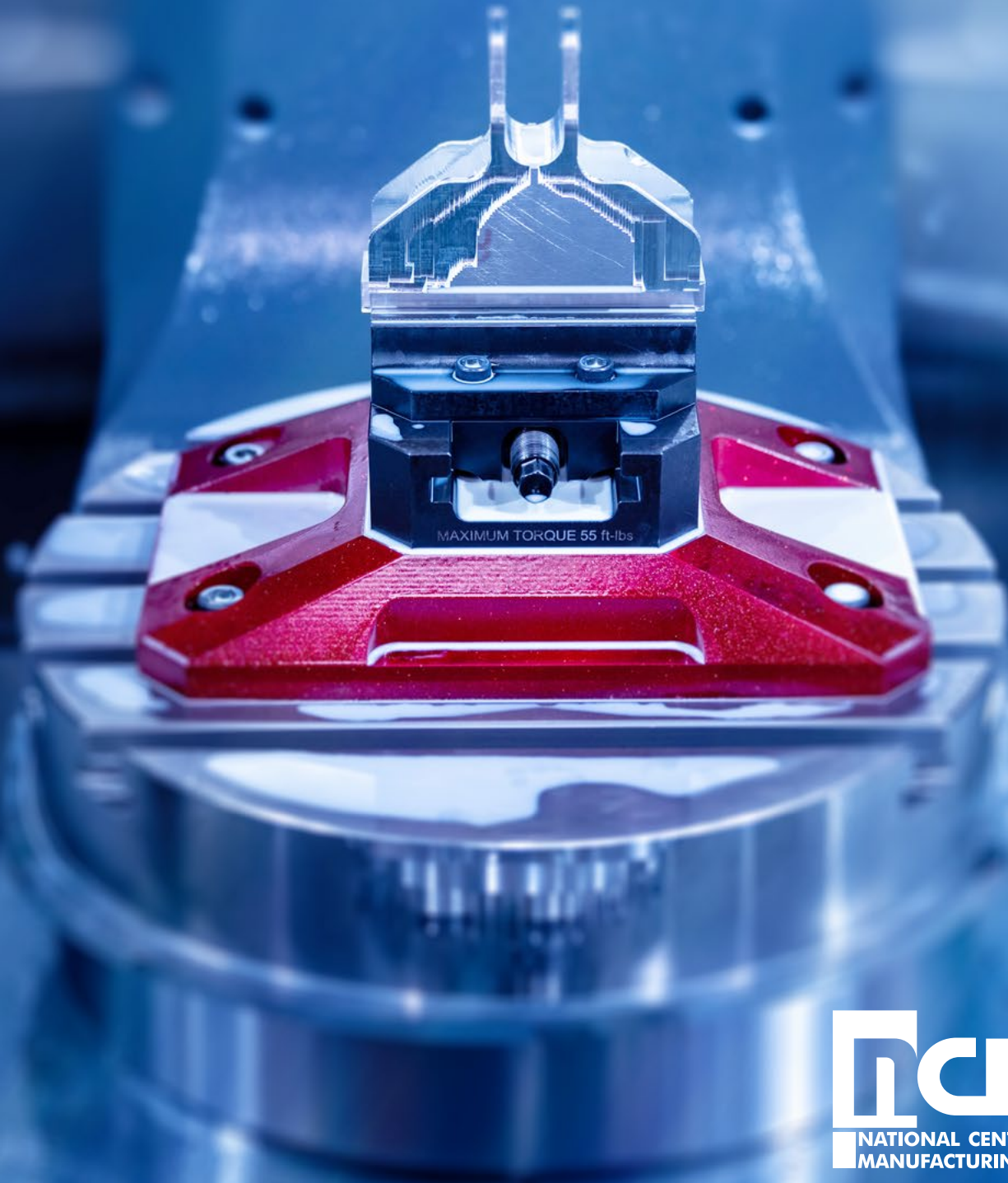


AI Workflows Significantly Reduce R&D Time for Innovations with Widespread Public Applications





Introduction

A recent [NCMS initiative](#) used hybrid human-AI workflows to significantly reduce R&D time for commercial and defense innovations. The research team built a machine learning (ML) model that, over a five-week period, supported the creation of several new high-performance adhesives capable of bonding plastic, steel, aluminum, and titanium. Utilizing AI to generate new options for adhesive chemistry was viewed as a possible route to solving a long-standing problem: Titanium is historically one of the most difficult metals to bond with adhesives. While titanium has many applications—consumer goods, medical and dental implants, and commercial and military aircraft components—adhesive bonding of titanium is a well-known manufacturing challenge requiring special surface preparation, such as chemical etching, anodizing, or grit-blasting.

Establishing an Experimental and Computational Foundation

The objective of this project was to create high-strength adhesives leveraging polyurethane and

polyurea chemistry. Made of different chemical bonds, polyurea cures in seconds and resists moisture during application, while polyurethane cures much more slowly and is easier to apply by hand. In this initiative, researchers investigated two-component polyurethane adhesives. These consist of two packages of ingredients prepared, then mixed, to form an adhesive. Researchers started with a formulation of conventional resins and varied the raw material package, evaluating different combinations of molecular weights and curing ratios, including the curing agent, curing agent-to-resin mix ratios, and curing temperatures.

The algorithm generated adhesive formulations that could be prepared in the laboratory and yield experimentally viable materials.

To discover new adhesive formulations, the team used an AI workflow, creating an algorithmic adhesives formulation generator. This algorithm incorporated several inputs acting as boundary conditions to ensure that formulations were chemically plausible and manufacturable. After training the algorithm with datasets, it generated adhesive formulations that could be prepared in the laboratory and yield experimentally viable materials. The algorithm rapidly generated 100,000+ unique, valid formulations with the total number limited only by the available time and computational hardware. Next, the team identified formulations likely to perform well in laboratory testing that were different enough from previous laboratory experiments and worth testing to learn something new.

Harnessing the Power of AI Workflows

The researchers used Bayesian machine learning (ML), which applies the principles of Bayesian probability theory to statistical modeling and pattern recognition. Traditional ML starts with inductive biases (structural choices made by engineers to help the model generalize) and random mathematical initialization. In contrast, Bayesian ML allows engineers to inject priors—existing domain knowledge, historical data, or physical constraints—into the algorithm before training even begins.

In this initiative, the researchers used a “human-in-the-loop” strategy. Each week, the ML model suggested 30 formulations; the researchers chose the 15 most likely to yield valuable and informative data. Chemists leveraged their expertise to run experimental tests and feed the performance data back into the model.

The substrates on which the team tested the adhesives were selected based on their popularity in the automotive industry. Methyl ethyl ketone (MEK) and isopropyl alcohol (IPA) were used as solvents due to their wide usage in manufacturing processes. The substrates included in this experiment were:

- MEK Al 6061 (0.8128 mm thickness), a 6061-

grade aluminum sheet, surface-cleaned with MEK

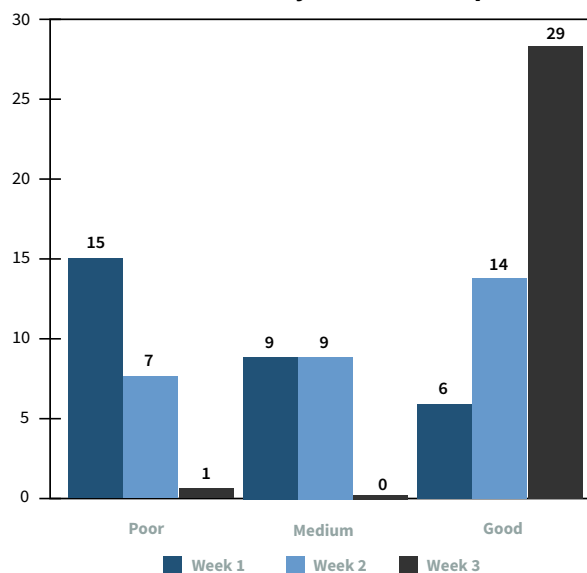
- MEK HDG (0.7874 mm thickness), a hot-dip galvanized steel sheet, surface-cleaned with MEK
- IPA PC-ABS 25% (3.175 mm thickness), a type of plastic—specifically a Polycarbonate-Acrylonitrile Butadiene Styrene (PC-ABS) polymer blend—surface-cleaned with IPA
- Titanium Grade 5 (Ti-6Al-4V)

Researchers carried out experimental evaluations via mechanical testing. The control used in the experiment was Aluminum 6061 with an adhesion promoter. To ensure consistent inputs into the ML model, the researchers standardized the preparation of samples, instrument procedures, and data collection.

The team’s AI workflow calibrated the ML model to generate formulations that optimized two key parameters. The first was lap shear strength, which is the measure of an adhesive’s ability to resist forces that try to slide two bonded surfaces past one another in opposite directions. Lap shear testing was conducted to understand the nature of the adhesive bond to the metal substrate and quantify the strength of adhesion.

The ML model also optimized percent cohesive failure mode—a quantitative metric that

Figure 1: Initial Iterative Improvement of Model with Increased Cycles of Development



measures the percentage of a fractured joint's surface area where the adhesive layer itself tore apart, rather than peeling away from the substrate. Metrics on both percent cohesive failure mode and lap shear strength are required in laboratory reports to meet American Society for Testing and Materials (ASTM) standards.

To train the ML model, the team categorized each formulation's mechanical performance as poor, medium, or good. A poor formulation meant the adhesive showed zero ability to adhere to the substrate and had poor mechanical performance. A medium formulation indicated the formulation had one or two potential issues (for example, high viscosity or imbalanced kinetics) that would hold back the formulation from performing to the best of its capability. Good formulations provided the most valuable and reproducible data points to feed the model.

Initially, the model was fed 7 good formulations, 5 bad formulations, and 3 medium formulations so that the model would be able to understand and define the performance of each type of formulation. In the second round, the model was fed 11 good formulations and 4 bad formulations. The model responded to experimental feedback very quickly. Within three weeks, the model significantly increased its output of good formulations and decreased its output of bad formulations (See Figure 1).

Results

After five weeks, the AI workflow created a set of adhesives capable of adhering to several important substrate materials. The ML model identified optimal adhesive chemistries that balance stiffness, toughness, and cure kinetics for high-load structural bonding. Additionally, the model provided predictive insights into key performance properties based on molecular structures and formulation parameters, reducing reliance on lengthy mechanical testing cycles.

Ultimately, the model yielded multiple formulations with acceptable direct-to-metal adhesion and lap shear strengths above 5MPa—an engineering performance threshold where an adhesive joint can withstand a parallel sliding force (shear stress) of at least 5 Megapascals,

which is equivalent to approximately 725 pounds per square inch (psi), before breaking.

An important finding was the beneficial role of aminic reactive resins in achieving direct-to-metal adhesion. Aminic reactive resins cross-link polymer networks to transform soft liquid mixtures into hardened, durable industrial materials. In this experiment, adhesive formulations containing aminic reactive resins consistently outperformed those without it. This insight provided valuable knowledge for both ongoing and future adhesive development.

In the final stage of the experiment, researchers tested the highest-performing adhesive formulations to determine whether they could bond directly to titanium samples without surface preparation. The differences in how each of the highest performing adhesives generated by the adaptive model adhere to aluminum and titanium are striking. The data clearly shows that despite an adhesive performing well on the aluminum substrate it does not necessarily mean that the performance translates to the titanium substrate. Results confirmed that at least one model-generated formulation exhibited strong adhesion on grade 5 titanium, historically one of the most challenging substrates for polyurethane adhesives.

Conclusion: Public Benefits of This Initiative

The titanium-bonding adhesive created in this project provides a unique engineering advantage: it combines the elasticity and impact resistance of a polyurethane with the ultra-high strength and lightweight properties of titanium. This adhesive could be used to improve medical and dental implants, create lighter and more efficient vehicles, reduce infrastructure costs, and produce more durable electronics. The entire set of adhesives developed in this initiative could be used in packaging, construction, automotive, electronics, consumer goods, furniture, healthcare, and beyond, unlocking widespread public benefits across multiple industries.

This project successfully demonstrated that an AI-enhanced design of experiments significantly

accelerates adhesive formulation research. Within a five-week period, the integration of ML, formulation generation, experimental feedback, and computational chemistry yielded multiple new adhesives, including a direct-to-metal titanium-bonding adhesive. The design of experiments used in this initiative can be replicated in adhesive development workflows to improve reproducibility, efficiency, and scalability. More generally, the project confirmed that hybrid human-AI workflows can meaningfully enhance R&D efficiency for both commercial and defense applications.

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