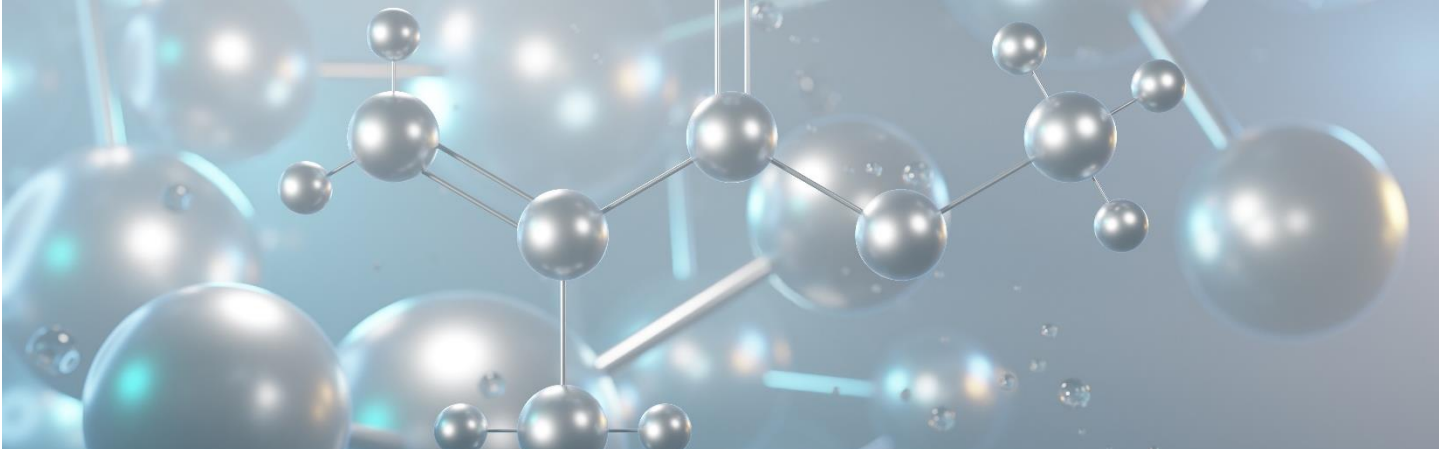


# REVOLUTIONIZING POLYMER DEVELOPMENT WITH ARTIFICIAL INTELLIGENCE



## Introduction

Material science has been a cornerstone of human innovation for millennia and is arguably one of the biggest drivers of technological breakthroughs. While there's plenty of research into the properties and behavior of materials and in material science generally, the development of new polymers represents a significant challenge in the field.

Polymers are complex materials made up of long chains of repeating molecular units called monomers. Their versatility comes from their diverse structures, which can be linear, branched, or cross-linked, giving rise to a range of properties. This complexity allows polymers to be tailored for countless applications, from flexible plastics to strong, lightweight composites. The behavior of polymers is influenced by many factors such as molecular weight, temperature, and chemical composition, making their study challenging. Yet at the same time, understanding these factors is essential for advancements in fields such as materials science, medicine, engineering, and more.

Thankfully, we can now use new advances in technology to innovate and find new novel materials faster than ever before. Artificial intelligence (AI) and machine learning, combined with advanced optimization algorithms, provide a new paradigm for material science. Whether it's increasing performance, reducing cost, or improving materials' recyclability, utilizing predictive and prescriptive analysis presents an exciting opportunity.

## The Challenge

For advanced engineering applications, new materials are often needed when the limits of known materials are reached. Too often, we may reach a point where existing materials don't meet the requirements of the environment they're used in. They might become brittle at lower temperatures or fail to show the required mix of ductility and strength that design engineers require.

At this point, material scientists will compare their requirements with known material compositions and use their best judgement to propose new mixtures. These new mixtures are then sent away and tested in a laboratory or external testing facility where they're tested to ensure statistically significant results. If one of the new material candidates meets the required conditions, it can be used for the new application. Otherwise, the cycle of creating and testing repeats. This approach poses two major challenges:

- 1. It can be very iterative, time consuming, expensive, and often relies on a large amount of testing** to reach a suitable candidate material. It also depends heavily on the experience of the material scientist to guide the process and ensure the search is successful.
- 2. Teams often struggle to determine if a material is the “optimal” solution**, even if all needed criteria is met. For example, perhaps the material could've performed even better with some fine-tuning of the material ratios; or maybe it could've been produced more cost effectively. Again, the limitations of time and cost using a traditional approach hinder the material development process.

## The Solution

While machine learning and AI usage have increased in recent years, the technology isn't currently used widely to innovate material development. The key barrier is the complexity of the AI and machine learning domains, which traditionally require a strong background in data science, coding, and material science. This is where the Altair® RapidMiner® data analytics and AI platform can help.

By enabling all users to participate in data science through a code-optional experience that caters to experts and novices alike, users of all levels can build powerful data and machine learning pipelines regardless of their data science expertise. Combined with Altair's rich heritage in using machine learning for optimization, this can enable predictive (like how well new material formulations will perform) and prescriptive insights. By this, we mean utilizing AI and machine learning models for optimization to propose novel material formulations that better meet design criteria. This way, companies can truly leverage the power of machine learning and AI to accelerate the discovery of novel materials.

## The Methodology

Developing new polymers with AI and machine learning is a complex and multifaceted process. We first require predictive machine learning models to predict material KPIs, based on the formulation and processing parameters. The data used to build these models is collected from the baseline performance of known materials and any tests already performed. Any data collection, preparation, and processing can be performed using point-and-click operations, or in visual workflows. An example of these visual processes is shown in Figure 1.

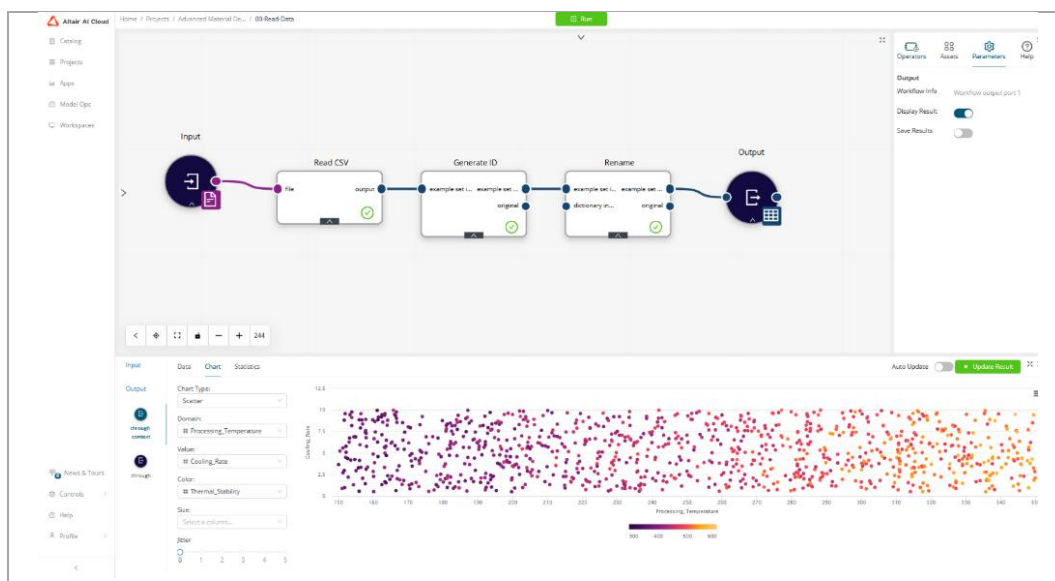


Figure 1 – Altair® AI Cloud Workflow Designer showing a data preparation process

Users generally want to prepare data for these applications into a neatly defined table with one or more target output columns and several input columns we want to use to make our predictions. Common preparation steps will include filtering out or replacing missing values, calculating new columns, conversion of data types, etc. All these steps are performed by adding new operators to visual workflows so users can efficiently perform quick, repetition-free prototyping.

Once the data is suitably prepared, users can begin to build machine learning models. These models, through the training process, will learn the relationship between the input data and target outputs, and users can utilize testing data to confirm that these models' predictions are accurate. A great place to start initial model training is by using AutoML; automatically training and testing a variety of common machine learning algorithms. Good data science practice is built in for the end user, meaning anyone with a dataset can immediately begin training machine learning models.

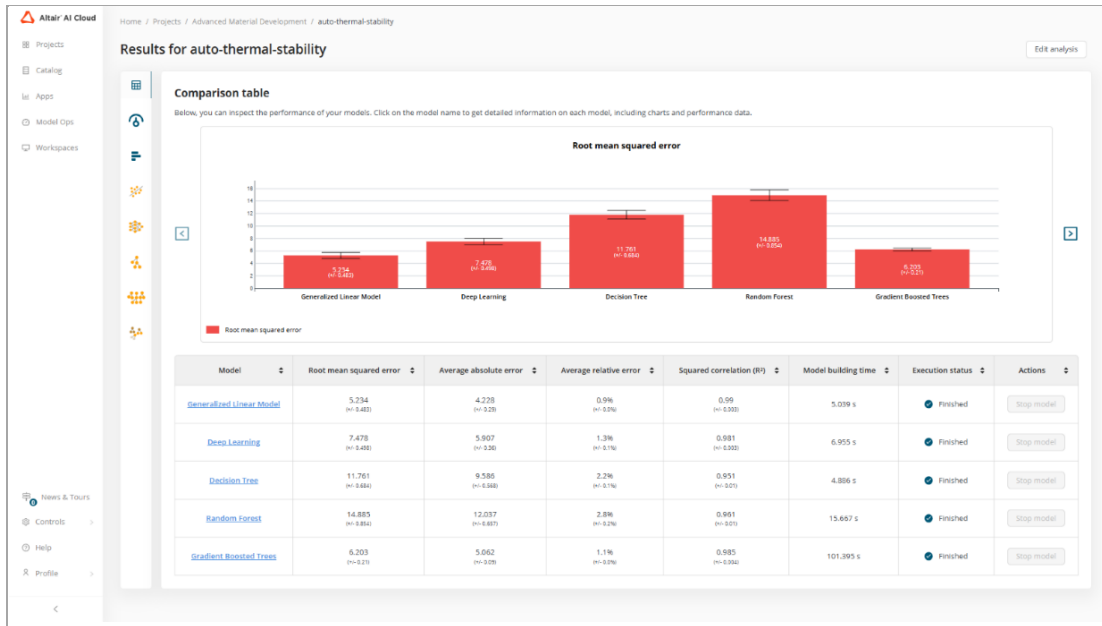


Figure 2 – AutoML results comparison view of the machine learning models trained

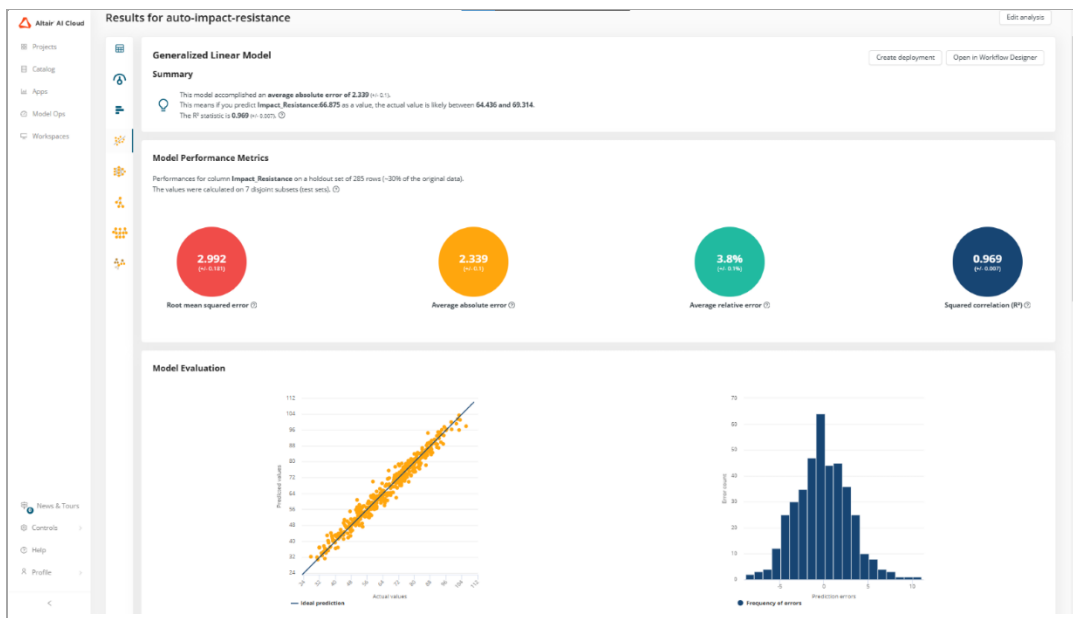


Figure 3 – Auto AI results for a generalized linear model

Common performance metrics such as accuracy or average error are automatically generated for the user, facilitating easy comparison between the different machine learning models. Users also have access to features such as weights – allowing quantitative rating of the importance of the input columns in getting a good prediction – and a model simulator where users can test new input values on the fly.

Once the user completes AutoML training, they can either immediately deploy one of the trained models or continue development with visual workflows or coding. For example, shown below is a workflow designed to train and optimize three separate machine learning models, where we evaluated dozens of candidates to find the best parameters for increasing model performance and accuracy.

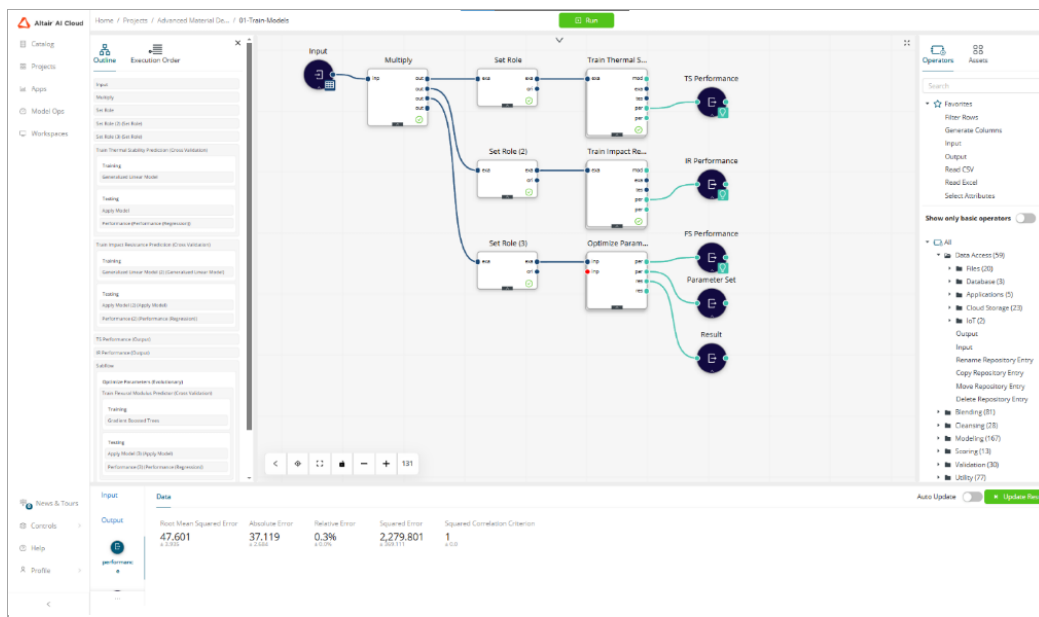


Figure 4 – Workflow Designer showing the training and optimization of three separate machine learning models

Once users are happy with the quality of their predictions, they must then consider how to transform predictive insights into prescriptive insights. This is where users are no longer just using AI to predict the performance of materials assigned input values, but where AI suggests inputs based off the values teams want to achieve.

We can frame this as an optimization problem in which we have KPIs we want our material to meet, along with constraints it must not exceed. This is the perfect application of Altair® HyperStudy®, a powerful multidisciplinary design exploration and optimization tool. Users can follow a guided step-by-step process to connect to a deployed model, set up the necessary parameters, extract the results that interest them, and utilize state-of-the-art mathematical models and data mining. All of this allows for a smarter, more robust exploration of possible material design combinations. HyperStudy provides flexibility that allows users to design advanced optimization solutions where they can optimize the inputs to their machine learning models; in other words, optimizing material design while optimizing for multiple objectives and considering real-world constraints.

Users integrate the trained model into HyperStudy, stating the inputs and how they wish to vary them. For numerical variables, users can choose whether to allow any value within a range, or discrete levels taking specific values. Similarly, users can choose the values for any categorical columns. One activity to initially try is a design of experiments (DoE), where the total possible collection of input options is sampled to give a broad understanding of the possible performance of a new material's design. Users then define the optimization problem they want to solve, setting any constraints – such as equal amounts or consistent ratios of two or more inputs – or ensuring a KPI doesn't fall below a certain threshold. Users can also set targets during this step. Finally, users can then set up the optimization by choosing an algorithm – such as a response surface method or genetic algorithm – and setting any optional parameters.

Once the optimization is complete, users can post-process the results to determine the best designs. When optimizing for two or more objectives, users can analyze the trade-offs between competing objectives and do any additional processing such as report generation or a comparison of the distance of the optimal points from known test results.

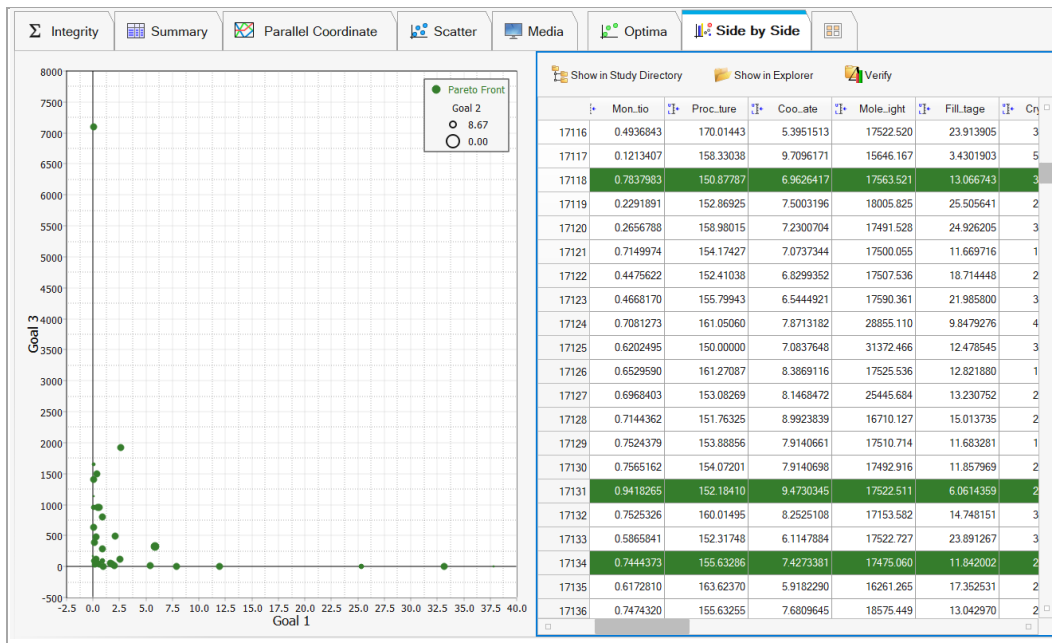


Figure 5 – Examining the new proposed materials with powerful post-processing tools

By following this workflow, teams can generate innovative new material candidates far faster than previously possible. Moreover, this process isn't limited to polymers; it can be utilized to generate a wide variety of materials. These workflows are reusable, so if users receive more data or want to apply the workflow to a new problem, the process can be re-run.

**Conclusion**

Altair uniquely combines expertise in data science, material science, and engineering with cutting-edge technology to deliver groundbreaking innovations. Unlike other providers that may only offer machine learning solutions, Altair advances beyond conventional material data science by leveraging prescriptive AI. This approach both analyses material data and recommends the optimal material composition to achieve defined performance targets.

Altair's integrated approach brings together solutions from its extensive portfolio into cohesive, powerful workflows designed to address organizations' most complex challenges. A key component of this ecosystem is the integration of the Altair RapidMiner platform with Altair® Material Data Center™. This synergy consolidates materials intelligence into a single source of truth, leveraging advanced machine learning models to drive innovation, bridge data gaps, and optimize material selection—all of which provide a critical competitive edge in achieving sustainable product innovation.

Best of all, what's shown here is only a glimpse of Altair technology's capabilities. For more information on Altair's technology capabilities and how they can help you redefine material intelligence for unparalleled innovation, visit [altair.com/altair-rapidminer](http://altair.com/altair-rapidminer) or [altair.com/materials](http://altair.com/materials).