

# ACCELERATING OPTIMIZED FORMULATION OF TIRES SCIENTIFIC DATA ANALYSIS AND MACHINE LEARNING

Datasheet

Product Development in the Industrial Equipment industry has always relied on speed and innovation. Companies extending from tire manufacturers to building equipment and from heavy mobile machinery and equipment to industrial robots and machine tools need to provide highly specific products to their customers and end consumers. Innovation and reliability, together with a high degree of support, are key for success in these industries. Looking specifically at tire manufacturing, important factors influencing this success are (1) the equipment needed to support the complex process of manufacturing a tire and (2) the formulation of the tire itself.

Specifically, two types of simulation play key roles in tire formulation development.

1. Atomistic simulations that can predict the properties of the rubber formulation that can then flow into the finite element (FE) simulation of a complete tire, which would, for example, allow scientists to assess tire grip on a wet road.
2. Simulation based on data models created from actual measured data of given physical formulations and measured parameters such as grip.

In the following we will focus mainly on the second concept.

If R&D teams can achieve the agility needed to rapidly develop new tire products or reformulate existing tires, they can gain a serious competitive edge. To do this, however, organizations need to embrace virtual approaches to R&D. Artificial Intelligence (AI) and Machine Learning (ML) offer a unique advantage over physical experimentation alone: scientists can leverage existing formulation data to predict and optimize the formulation of new tire products based on desired end properties. This can help R&D teams focus more time- and resource-intensive lab work on projects that are more likely to succeed.

## VIRTUAL PRODUCT DESIGN AND OPTIMIZATION

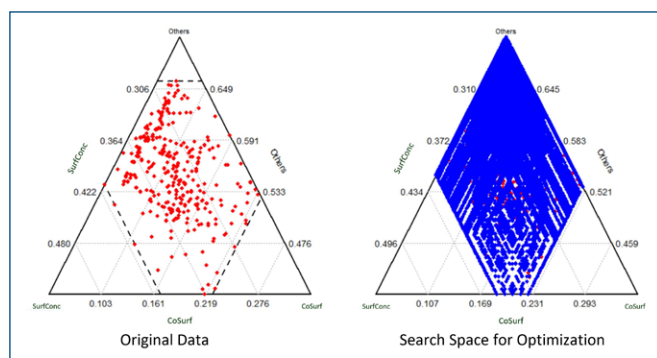
BIOVIA's solution for Scientific Data Analysis and Machine Learning provides comprehensive capabilities for formulation development and optimization for tires. It brings together decades of data science experience to allow data scientists to aggregate and clean data, train and validate models, and share and deploy complete workflows to researchers at the enterprise level.

The solution supports data-driven decisions for tire manufacturers from product design through development to commercialization. In research and development, optimization algorithms help to enhance new rubber recipes. Based on the ingredients in the recipe, these algorithms can predict properties of the finished material such as viscosity and grip, as well as the formula's temperature-dependent performance. Digital flow charts help scientists decide when to proceed with physical experiments and which formulation has the best chance of achieving the new planned performance parameters. Overall, these Machine Learning tools help tire manufacturers to develop new formulations meeting particular specifications faster, while also helping them to decide if it is worth the investment to bring a new formulation to market.

## SIMPLIFYING MULTI-OBJECTIVE OPTIMIZATION

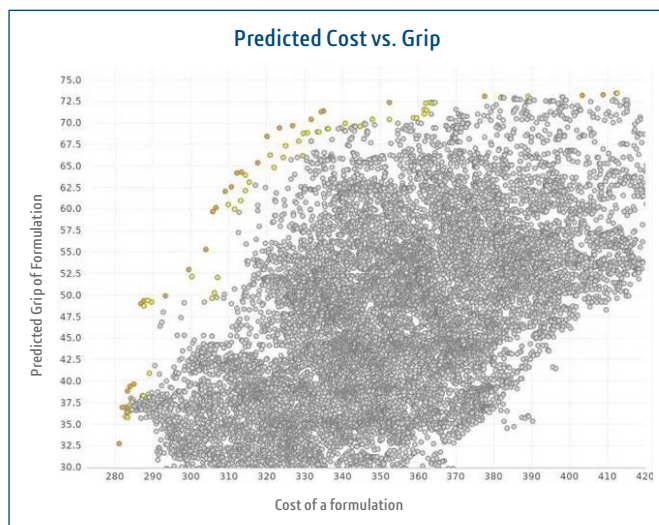
In designing formulated products, scientists must effectively tie chemistry to product performance, which is a familiar R&D challenge. For example, winter tires need to be flexible at lower temperatures. Summer tires need to be rigid at high temperatures and high speed. Both attributes source their properties from the ingredients of the tire formulations.

BIOVIA's Scientific Data Analysis and Machine Learning solution allows formulation chemists to leverage existing product data to drive new tire formulations. Data scientists can clean and curate product performance datasets to train machine learning models that can predict product behavior such as viscosity of the formulation or glass temperature of polymers based on their formulations. Product developers can then take a Design of Experiment (DoE) approach to define a design space for new formulations, which can then be "tested" by the model (Figure 1). Finally, teams can utilize methods such as Pareto sorting to identify optimal formulations, based on their desired characteristics, to make and test in the lab (Figure 2). For maximum efficiency in speeding successful product to market, product developers like to focus their bench work on formulas that are most likely to succeed.



**Figure 1.** A visualization of a three component mixture. Product Developers can use this Design of Experiment approach to constrain a Machine Learning model which predicts the behavior of various tire formulations.



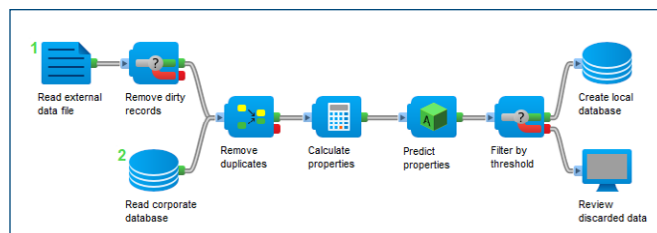


**Figure 2.** Pareto optimization of various tire formulations finds the ‘best’ predicted recipes (in blue) based on multiple design objectives (Costs vs. Grip). Researchers can focus subsequent lab work on these optimal suggestions.

## GROUNDING IN SOUND DATA SCIENCE

The creation of any model, no matter how complex, requires solid fundamentals to succeed. Data scientists need to continuously curate high quality data sets, while generating and validating models to ensure that end users can trust them. The Scientific Data Analysis & Machine Learning solution is based on BIOVIA Pipeline Pilot, which offers a complete collection of tools and methods to help scientists and formulators rapidly create targeted data science applications for their organization. With BIOVIA Pipeline Pilot you can:

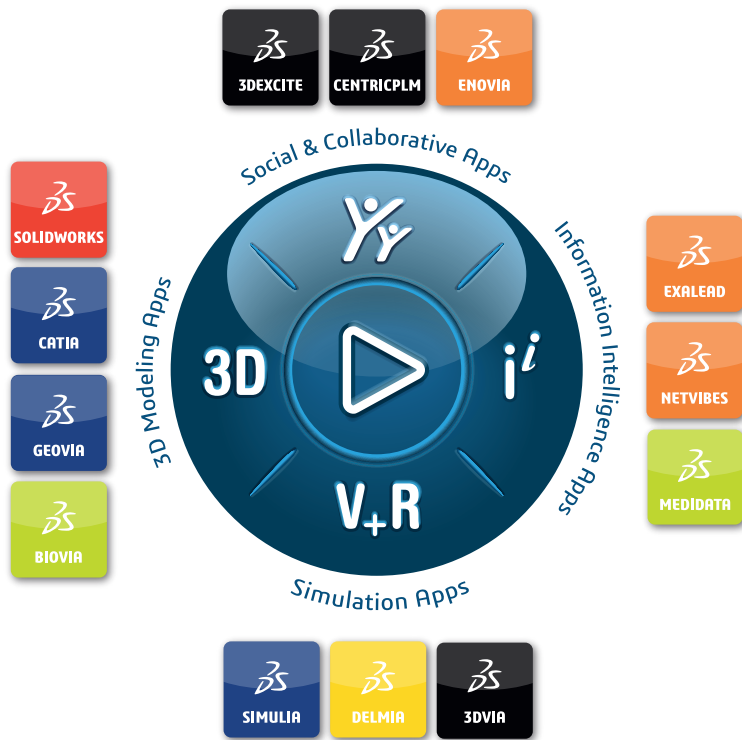
- Automate data access, curation and cleaning prior to model training and validation
- Accelerate the creation of complete workflows via a low-code/no-code graphical user interface
- Use prebuilt architectures for random forest, genetic functional algorithms and neural networks or import custom Python scripts and libraries
- Integrate functionality developed with Jupyter Notebooks, Anaconda, and TensorFlow
- Configure the reporting and exporting of results
- Rapidly deploy models and workflows across various teams or the entire enterprise as web services or custom applications



**Figure 3.** An example data science workflow within BIOVIA Pipeline Pilot. This solution provides the backbone for the Scientific Data Analysis & Machine Learning solution. It utilizes a graphical user interface to simplify and accelerate the creation of complete tools for various data science use cases.

## BRINGING OPTIMIZED OFFERINGS TO MARKET, FASTER

Maintaining R&D agility is not just a tactic to keep pace with the market; it can become a key competitive differentiator. By adding advanced machine learning techniques to physical experimentation, tire manufacturer teams can maximize the value of their previous work and accelerate the next phase of tire development. The Scientific Data Analysis and Machine Learning solution from BIOVIA facilitates this transformation in tire formulation. With it, teams can better target their work and increase productivity by focusing on science-led innovation. They can decrease R&D costs by reducing physical tests and speed reformulation by complying with regulatory and environmental demands while also providing new product properties more quickly. Tire manufacturers can capitalize on their long-term knowledge and intellectual property, ultimately speeding the most promising new tire products to market.



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