NOBLEAI

USE CASE

Reformulating Polyurethanes with More Sustainable Chemistries

Enhance polyurethane performance using predictive chemistry inside Noble Reactor.

Target

Polyurethanes are an exciting material class with limitless potential enabled by combinations of new monomer chemistries.

How does one choose from the growing portfolio of new, sustainable chemistries being developed?

Challenge

Polyurethanes have a combinatorial design space across new chemistries and processing conditions. While processing conditions are amenable to optimization via classical design of experiments, optimization across monomer chemistries is a much more challenging, uncertain, and costly task.

Forecasting the performance of new monomer chemistries can reduce the risk of exploring and accelerate the design of next generation polyurethane materials.

Solution

Configure NobleAI Reactor to predict the mechanical properties of new polyurethane materials across many processing conditions and monomer choices.

Reactor's science-based ML models can account for kinetic reactivity and augment physical characterization of materials to provide structural insight into the performance of polyurethane materials. These insights in turn can drive understanding of how chemistry and processing conditions drive meso-scale structure and material performance.

Reactor has optimization algorithms that can suggest monomer chemistries, facilitating search through existing commercially available monomers, or advancing the design of novel monomers.