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PFAS Replacement Analysis Use Case

Alternatives to the perfluoropolyether (PFPE) alcohol component via Replacement Analysis in LabDX

PFAS Replacement Project

This project focuses on replacing PFAS-based materials in colonoscopy tubing with safer, non-fluorinated alternatives while maintaining critical surface performance.

The project objectives:

maximize water contact angle
- enhancing hydrophobicity to reduce biofouling and fluid adhesion

minimize kinetic friction
- ensuring smooth insertion and maneuverability within the colon

Data: **no in-house experiments** available.

Our solution: curated **28 patents** relevant to PFAS replacement problematics focuses around contact angle and kinetic friction.

PFAS Replacement: Model Finetuning - Water Contact Angle

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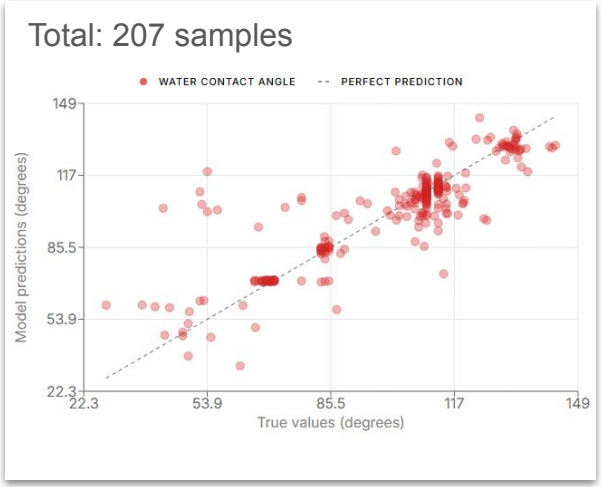
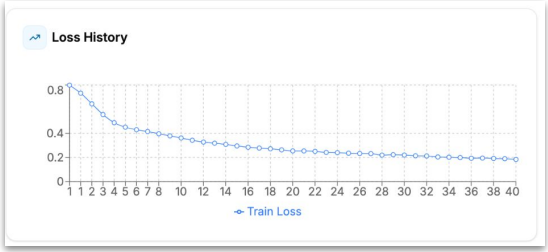
Base model provides **general context**. At the same time, customer needs **high precision for a specific task**. To meet this requirement, we use customer data to fine-tune an individual copy of the base model.

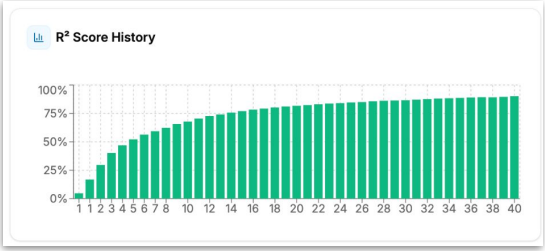
The resulting model shows good performance even on very limited datasets.

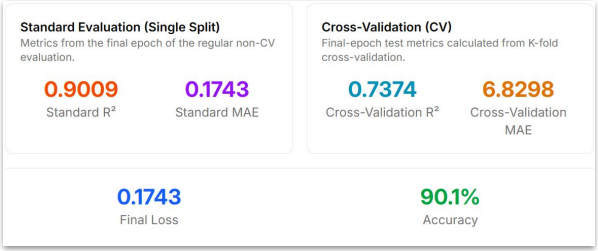
> ***The plot shows a strong correlation between predicted and actual water contact angle values despite data variation.***

Water contact angle fine-tuning based on 28 curated patents









PFAS Replacement: Model Finetuning - Coefficient of Kinetic Friction

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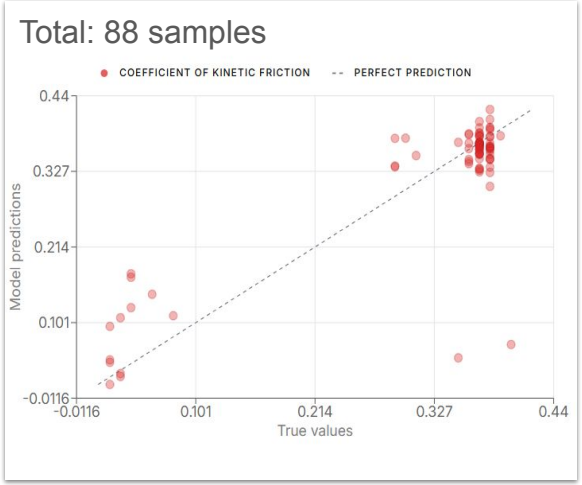
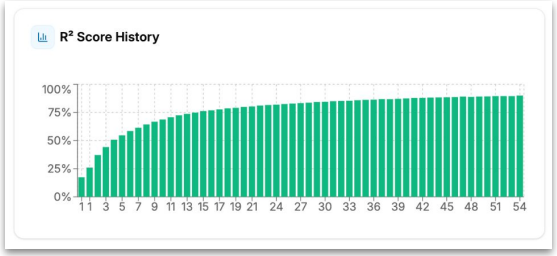
Base model provides **general context**. At the same time, customer needs **high precision for a specific task**. To meet this requirement, we use customer data to fine-tune an individual copy of the base model.

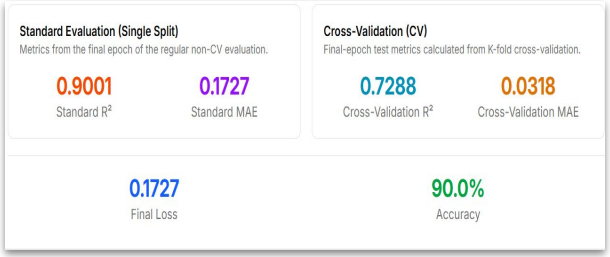
The resulting model shows good performance even on very limited datasets.

> ***The plot shows a strong correlation between predicted and actual coefficient of kinetic friction values despite data variation.***

Coefficient of kinetic friction fine-tuning based on 28 curated patents







Patent Overview

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Reference Patent

↳ Refer to patent link here

Patent ID	US-9982084-B2	Patent Title	Surface treatment composition	Assignee	Daikin Industries Limited

Properties of Interest

Water contact angle	Defined as the angle formed between a liquid droplet and a solid surface ❖ Indicates the wettability of the surface and its hydrophobic or hydrophilic characteristics based on intermolecular interaction [>90° = hydrophobic; <90° = hydrophilic]
Coefficient of kinetic friction	Quantifies the friction intensity of a sliding surface relative to another ❖ Low values mean surfaces slide easily with minimal resistance; high values indicate a greater resistance to motion

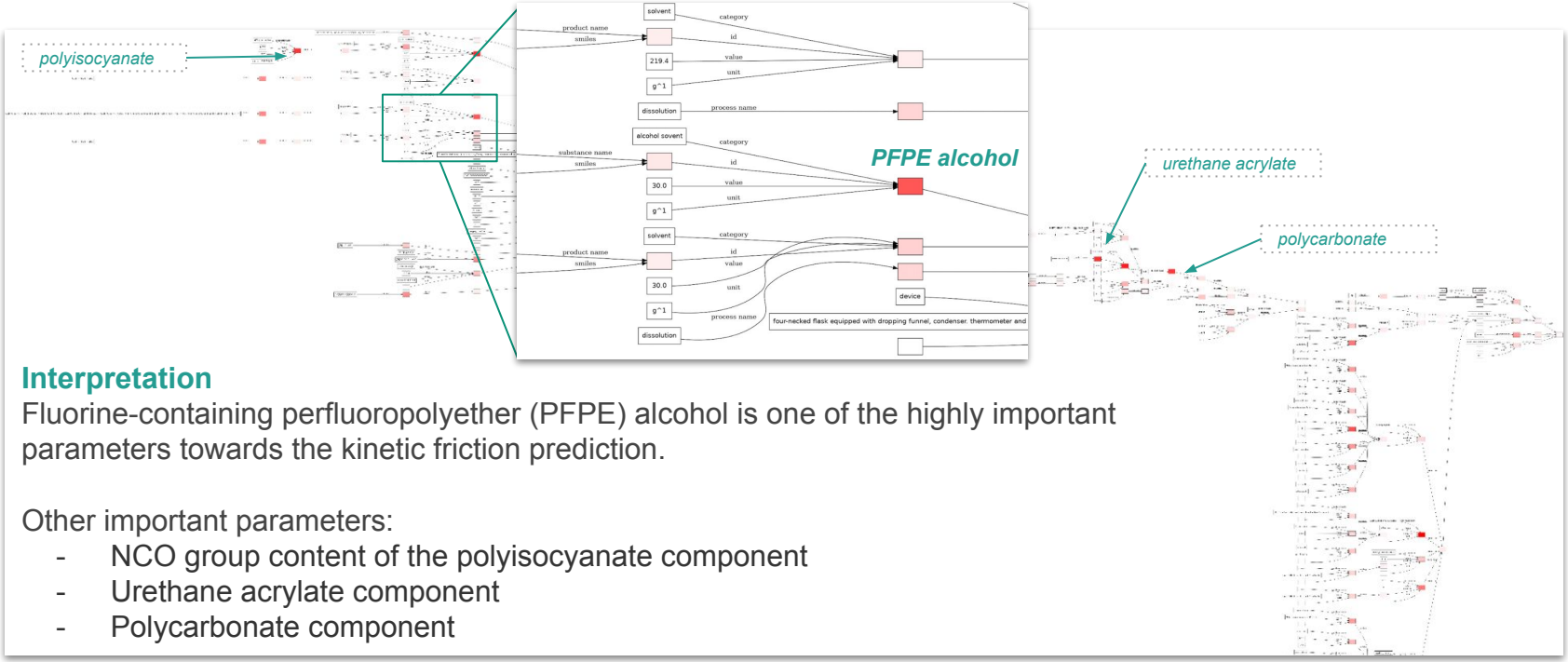
Materials

polyisocyanate | perfluoropolyether with an active hydrogen | silane compound with an active hydrogen | monomer having an active hydrogen

Factor Analysis | Coefficient of Kinetic Friction

Visualizing key elements influencing the formulation using GradCAM Factor Analysis:

- Each node represents a material, parameter, or process condition
- The intensity of the color signifies the model's focus or attention



Interpretation

Fluorine-containing perfluoropolyether (PFPE) alcohol is one of the highly important parameters towards the kinetic friction prediction.

Other important parameters:

- NCO group content of the polyisocyanate component
- Urethane acrylate component
- Polycarbonate component

PFAS Replacement: Replacement Analysis

Step 1: Extract candidate materials from our company's proprietary product database relevant for PFPE alcohol replacement

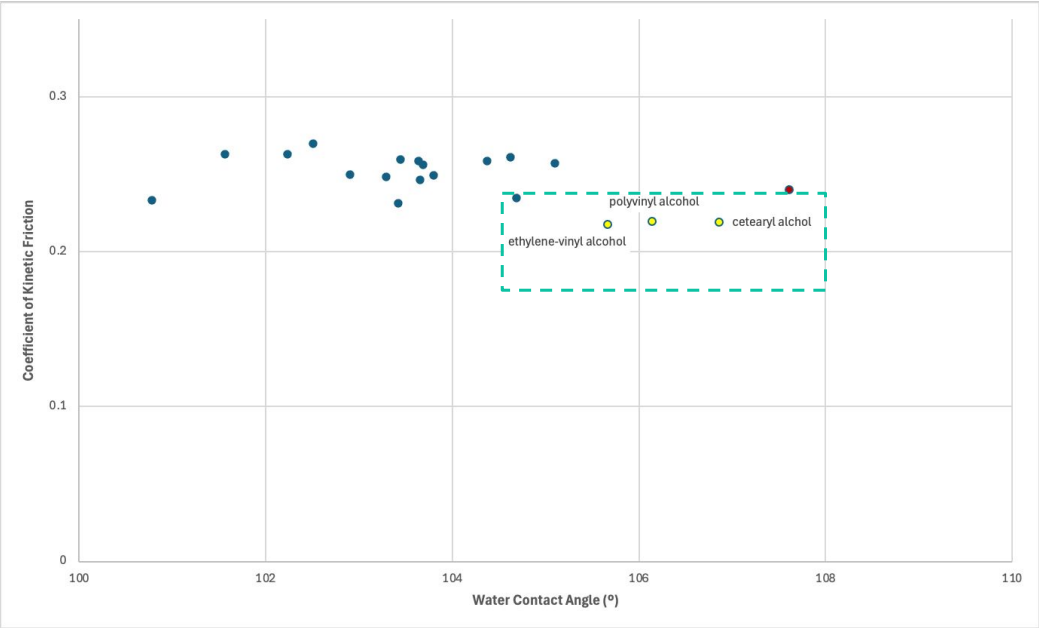
Step 2: Evaluate the synthetic candidates with the fine-tuned model on **water contact angle**

Step 3: Evaluate the same data with the fine-tuned model on **coefficient of kinetic friction**

*The two plots showcase the **property prediction results** when candidate materials from our catalog replace the original material in the original composition.*

PFAS Replacement: Replacement Analysis

Extract candidate materials from our company's proprietary product database and replace them in highlighted areas of high attention.



Substance name	water contact angle (°)	coefficient of kinetic friction
cetearyl alcohol	106.863702	0.21895212
polyvinyl alcohol	106.141748	0.21941727
ethylene-vinyl alcohol	105.667261	0.2175227

In the ranking of prediction results, **formulation candidates that balance both properties were extracted at the top.**

In this replacement analysis, perfluoropolyether (PFPE) alcohol was chosen as the material to be replaced with alternative candidate components.