TU Clausthal

Kolloquium zur Masterarbeit

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"Investigation of Explainable AI Methods for Polymerisation Process Modelling "

Polymers are macro-molecules composed of the monomer building block. These raw materials have numerous technical applications. They have a wide range of properties that can be tailored by the type and the conditions of the production process, ideally by modeling the polymerization process. We propose ML models to investigate polymerization process properties, covering integrated polymerization process modeling and reverse engineering of the polymerization process. We use an open-source KMC simulator, "mcPolymer," and NextFlow scripting language to generate fast parallel processed and reproducible data for the ML methods. We have considered the vinyl acetate monomer and a batch polymerization process in our experiments.

We use a multi-target regression approach to predict multiple dependent outputs parallelly. We compare the performance of various ML methods: multivariate linear regression, decision tree, random forest, extra trees, AdaBoost, and gradient boost using R2, RMSE, and MAE metrics. As most of the considered ML methods are "black box" decision-tree-based ensemble methods, we explain the created models with various explainability techniques.

The main results of this investigation are: (1) a suite of ML models for the prediction of monomer conversion, molecular weight distribution (MWD) parameters, and shape. (2) an ML-based single-objective optimization approach for reverse engineering of polymerization processes, the process of determining the initial recipe, and the reaction time moment for a given MWD shape; (3) a clustering-based multi-objective optimization strategy for a given MWD shape, maximal monomer conversion and minimal reaction time.

The experimental results show that ML methods (random forest, extra trees) can predict monomer concentration, MWD parameters, and shape and reverse engineer with adequate performance (R2 > 0.95), even with a considerable decrease in training set size (50%). The input variable importance corresponds to the chemical experts' expectations. The reverse engineering optimization strategy produces optimal initial recipes.

Mittwoch, 30.11.2022, 09:00 Uhr

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