Statistical Modeling of Physical Foam Extrusion of PLA with Carbon Dioxide

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Polylactic acid (PLA) is a bio-based polymer synthesized from starch-derived components and composts at controlled industrial conditions of 60 °C producing carbon dioxide (CO2) and water only. Replacing fossil-based polymers, PLA is already used as biocompatible material in medical applications, as lightweight yet durable packaging material, and as thermal or sound insulation material, depending on its pores, morphology, and size distribution. Physical foam extrusion using CO2 produces PLA foams free of harmful byproducts with tunable properties. Simultaneously, compressed CO2 decreases the melting point of PLA, leading to a more economical process. Thus, PLA foams are customizable materials, independent of limited fossil resources, ready to be integrated into a sustainable closed-carbon-cycle economy, and satisfying the growing demand for high-performance yet environmentally friendly polymers. A previous study [1] reported on the physical foam extrusion on a planetary roller extruder plant for two types of PLA. The influence of extrusion parameters on porosity, pore structure, and degree of crystallinity of the resulting foams was analyzed. However, for widespread applications and mass production of PLA foams for varying applications, the foaming process has yet to be optimized, and its product properties are mapped as a function of controllable process parameters. This research aims at generating fast to compute statistical models predicting product properties of PLA foams. The models are analyzed to optimize product properties and manufacture target products. Usually, optimization requires experiments for all combinations of process parameters or CFD simulations of mechanistic models. Statistical modeling is an alternate, data-driven approach, requiring fewer resources and computational power. In statistical modeling, processes are seen as black-boxes, described only by inputs and correlated outputs, the process parameters, and product properties respectively. Knowledge about underlying physics is not necessary, as the models consist of mathematical functions or algorithms fitted to precisely describe the data, but can predict outcomes for unknown inputs with similar precision. From these predictions, input parameters for target product properties can be derived. Still, the quality of each model strongly depends on the available data as unrepresented influences are unrecognized, leading to inaccurate or false predictions.

In this work, the Regression Learner App from the Statistics and Machine Learning toolbox MATLAB is used to train different statistical models and machine learning algorithms on existing data. The app features linear regression models, regression trees, support vector machines, Gaussian process regression models, and ensembles of regression tree models. All of them are trained in the app on the full data samples of both 31 and 34 experimental runs for PLA 8052D and PLA 2003D, respectively. During training, data is loaded into the app while predictor variables of temperatures, pressures, and mass flow as well as the chosen target property and models of interest are chosen. Five-fold cross-validation is used to prevent overfitting. Foam diameter, foam density, porosity, average pore size, and pore density are modeled individually, training all available models three times. For each property, the model with the lowest root-mean-squared-error (RMSE) and the highest regression coefficient (R2) is chosen. In this work, support vector regression as well as Gaussian process regression, achieve the highest prediction quality but show slight changes in each new training. For PLA 8052D, averaged RMSE divided by the average property value range from 9,8 % to 106,8 % and R2 values range from 0,54 to 0,77. For PLA 2003D, averaged RMSE divided by average property value range from 2,3 % to 74,88 % and R2 values range from 0,4 to 0,67.

As the models do not predict all outcomes accurately, the quality of the data will be improved defined by Design of Experiment principles, and hyperparameters will be further optimized. The results of this research should contribute to the optimization of physical foaming processes in industrial applications and the appropriate choice of statistical models for similar processes.

[1] Winck, Judith (2021): Über Strömungen und Mischvorgänge im Planetwalzenextruder für die Schaumextrusion. 1. Auflage. Düren: Shaker (Berichte aus der Verfahrenstechnik). ISBN: 978-3-8440-7779-7