Smart Design of Thermoplastic Vulcanizate Products: Linking Process to Performance via Machine Learning

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Thermoplastic vulcanizates (TPVs) represent a very interesting material choice for many industrial applications due to their light weight, recyclability, design flexibility, and ease of processing by injection molding process [1, 2]. TPVs are composed of a high amount of crosslinked rubber particles dispersed in a thermoplastic matrix, and they are aimed to replace traditional, non-recyclable thermoset rubbers.

Efficiently designing TPV-based products presents significant challenges due to their nonlinear mechanical behavior and inherent heterogeneity. The mechanical properties of these materials are strongly influenced by their microstructure and the injection molding process parameters [3]. Additionally, the shearing stresses encountered during injection molding can introduce anisotropic characteristics, further complicating the prediction and optimization of their performance [4]. Current commercial simulation tools for injection molding are inadequate for accurately capturing the unique attributes of TPVs and the intricate interactions among processing conditions, microstructure, and material properties, thereby limiting their utility in product development.

The rise of artificial intelligence, “big data”, and the fourth paradigm of science, — which emphasizes data-driven discovery [5] — offers a promising path to tackle complex challenges in science and engineering. Machine learning (ML), encompassing data-driven regression and optimization algorithms, enables the modeling of complex relationships between injection molding parameters and material performance. Materials informatics, which merges ML with materials science, has demonstrated significant potential for material property prediction and establishing process-structure-property linkages [6, 7].

This study evaluates the use of ML to identify key injection molding parameters that influence the mechanical properties of TPVs and enable accurate prediction of stress-strain behavior for product design. In this context, interpretable and explainable ML models are sought to foster the adoption of data-driven methods in the industry.

To generate the training dataset, a full factorial design of experiments (DOE) was conducted, producing 32 TPV plaques under varying processing conditions. Dumbbell-shaped specimens were prepared from the middle and end regions of each plaque in both the transverse and longitudinal flow directions. Cyclic tensile tests were performed to measure two target properties: stress at 30% strain and the residual strain obtained after unloading from the 30% strain cycle. This procedure resulted in a database of 128 samples.

ML models with varying levels of complexity and interpretability (linear regression, decision trees, random forests, gradient boosting algorithms, and neural networks) were assessed to predict target mechanical properties using a rigorous evaluation protocol based on *k*-fold cross-validation and group splitting.

Random forests exhibited performance equivalent to that of more advanced models, achieving relative errors below 10% in almost 90% of predictions for both stress and residual strain (Figures 1 and 2). SHapley Additive exPlanations (SHAP) were used to interpret the models, revealing the most influential injection molding parameters (Figure 3).

These findings highlight the potential of ML for correlating injection molding parameters and TPV mechanical properties, ultimately streamlining the TPV product design and development workflow.

References

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Figures

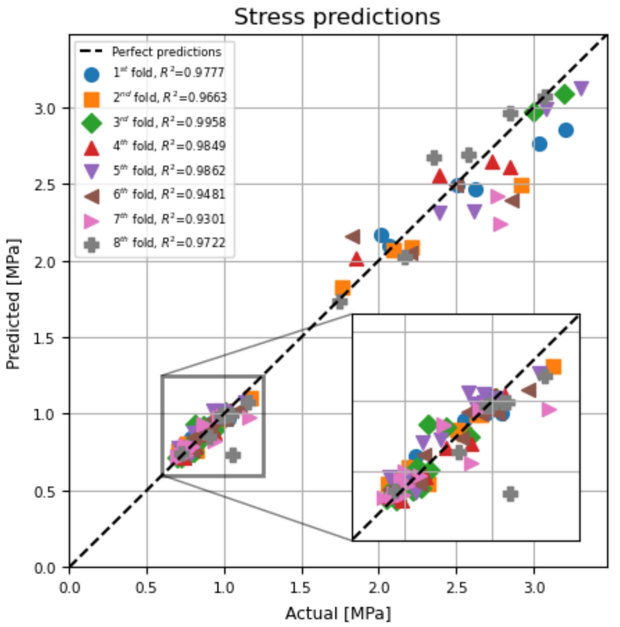

Figure 1. Parity plot illustrating the performance of the Random Forest model in predicting stress at 30% strain cycle, with results from the different cross-validation folds.

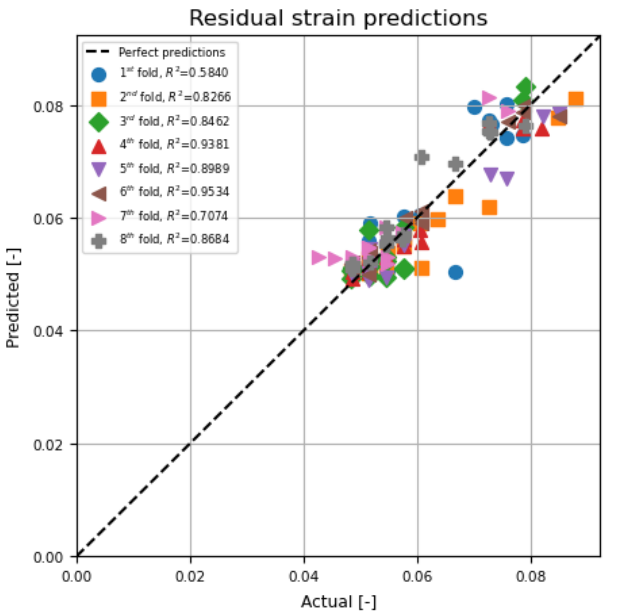

Figure 2. Parity plot illustrating the performance of the Random Forest model in predicting residual strain at 30% strain cycle, with results from the different cross-validation folds.

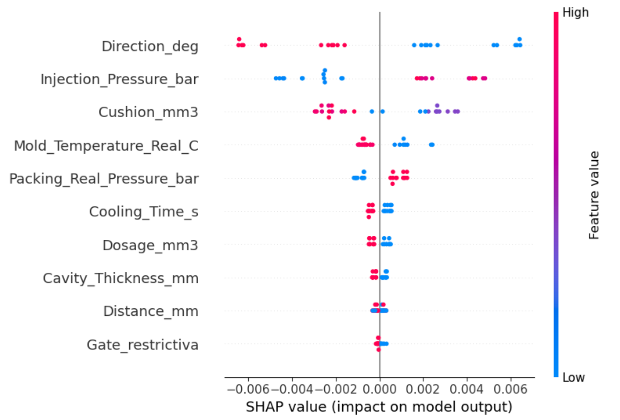

Figure 3. Feature importance and impact analysis using SHAP in the Random Forest model.