Machine learning-based surrogate modeling for efficient prediction of Moldex3D injection molding

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Abstract. Injection molding simulations using Moldex3D are essential for optimizing polymer processing, but they are often time-consuming and computationally expensive, especially when evaluating multiple materials and process conditions. This study examines the utilization of machine learning (ML) to accelerate simulation workflows by predicting key Moldex3D outputs without running full simulations. Two ensemble learning models–random forest (RF) and gradient boosting (GB)–were trained on simulation data from two polymer materials and used to predict three critical parameters for a third material, PP Domolen: filling time, packing sprue pressure, and warpage total displacement. The models' performance was assessed with mean absolute error (MAE) and root mean squared error (RMSE). Quantitative results indicate that the RF model attained an MAE of 0.151 seconds for filling time and 3.409 MPa for packing pressure, closely matching the actual Moldex3D values. GB performed better in predicting warpage, with an MAE of 0.762 *mm*, compared to 1.094 *mm* for RF. These results demonstrate that ML models can provide accurate predictions with significantly reduced computational time. This approach offers a promising step toward real-time optimization in polymer engineering and supports the broader adoption of AI-assisted manufacturing.

1 Introduction

Injection molding is a key element of polymer fabrication, commonly used to create complex parts with high accuracy and consistency. Simulation tools like Moldex3D are essential for optimizing process settings and predicting part quality, including important outcomes such as filling time, packing pressure, and warpage [1]. However, these simulations often require significant computing power, taking several hours to complete, especially when testing multiple materials or adjusting process conditions. This time requirement can slow product development and reduce the flexibility of industrial decision-making [2].

To address these challenges, researchers are increasingly turning to ML to speed up simulation workflows. ML models can learn from existing simulation data and predict outcomes

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for new materials or process settings, providing a faster and more flexible alternative to traditional simulations. For example, the authors in [3] demonstrated that combining explainable AI (XAI) with multistage transfer learning decreased the need for experimental and simulation data by up to 64%, while maintaining high prediction accuracy for optical lens quality.

Similarly, authors in [4] demonstrated that ML algorithms like neural networks and decision trees can predict injection molding quality with over 90% accuracy, even with limited training data. These methods are instrumental in industry 4.0 environments, where real-time data and smart manufacturing systems require quick and reliable insights.

In the field of polymer science, boosting algorithms like GB and XGBoost have become powerful tools for modeling complex, high-dimensional data. The authors of [5] reviewed the use of these models for predicting material properties, optimizing processing parameters, and designing polymer formulations, emphasizing their ability to capture non-linear relationships and improve prediction accuracy.

Building on this foundation, our study examines the use of RF and GB models to predict Moldex3D simulation outputs for a third polymer material, PP Domolen, using training data from two previously simulated materials. We focus on three key parameters: actual filling time, packing sprue pressure, and total displacement of warpage [6]. By comparing predicted values with actual simulation results, we aim to demonstrate that machine learning can significantly reduce simulation time and computational costs, while supporting data-driven decisions in polymer process optimization [7].

2 Methodology

This study aims to predict key injection molding simulation outputs–filling time, packing sprue pressure, and warpage total displacement–using machine learning models trained on Moldex3D simulation data. The methodology consists of four main stages: data preparation, model selection, training and validation, and performance evaluation.

2.1 ML models

2.1.1 RF algorithm

RF is an ensemble algorithm that enhances predictive performance and mitigates overfitting by aggregating the results of numerous decision trees. Each tree is trained on a bootstrapped data subset and considers only a random selection of features for every split [8].

Prediction function: For regression problems, the final prediction of a RF is computed by averaging the predictions of all its constituent decision trees:

$$\hat{y} = \frac{1}{T} \sum_{t=1}^{T} h_t(x) \tag{1}$$

where:

- T: the trees total number,
- $h_t(x)$: the prediction of the t^{th} decision tree,
- x: the input feature vector.

Each tree is trained independently, and the randomness introduced in sampling and feature selection helps reduce correlation among trees, improving generalization.

Feature importance (Mean decrease in impurity (MDI)): Feature importance in RF is calculated using the MDI:

$$FI_j = \sum_{t=1}^{T} \sum_{n \in N_j^t} \frac{\omega_n \Delta i(n)}{\sum_{n \in N^t} \omega_n \Delta i(n)} \tag{2}$$

where:

- FI_j: the importance of feature j,
- N_j^t: the nodes in tree t where feature j is utilized,
- ω_n: the samples number attaining node n,
- $\Delta i(n)$ represents the reduction in impurity achieved at node n.

2.1.2 GB algorithm

GB is a sequential ensemble technique that creates models iteratively. Every new model is trained to minimize the error (residuals) of the prior model using gradient descent on a loss function.

Prediction function: The latest prediction is the sum of the initial model and all subsequent corrections:

$$F_m(x) = \gamma_m h_m(x) + F_{m-1}(x) \tag{3}$$

where:

- $F_m(x)$: the model after m iterations,
- $F_{m-1}(x)$: the prior model,
- $h_m(x)$: the weak learner (characteristically a decision tree) trained on residuals,
- γ_m: the learning rate (controls step size).

Loss function minimization: GB minimizes a differentiable loss function $L(y, F(x))$, such as MSE:

$$L(y, F(x)) = \frac{1}{n} \sum_{i=1}^{n} (y_i - F(x_i))^2 \tag{4}$$

where:

- y_i: the actual value,
- $F(x_i)$: the predicted value from the model,
- n: the number of samples.

Gradient descent principle: GB minimizes the loss function using gradient descent, a method that iteratively adjusts the model to reduce error. At every iteration m, the model calculates the negative gradient of the loss function according to the actual prediction:

$$r_i^{(m)} = -\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} \tag{5}$$

These residuals $r_i^{(m)}$ represent the direction and magnitude of the error for each sample. A new weak learner, often a decision tree, is fitted to the residual values.

2.2 Data preparation

The dataset was constructed using Moldex3D simulation results for two polymer materials. Each data point includes:

- Geometric features: part thickness, flow length, gate location.
- Thermal features: melt temperature, mold temperature.
- Process parameters: injection speed, packing time, cooling time.

The target outputs for prediction were:

- Actual filling time (s).
- Packing sprue pressure (MPa).
- Warpage total displacement (mm).

The models were trained to predict these outputs for a third material, PP Domolen, using the features extracted from the simulations of the first two materials [9][10].

2.3 Model training and validation

A 80/20 train-test split was applied to the dataset. Subsequently, the hyperparameters for both models were tuned via grid search with cross-validation. Feature importance is detailed to understand which parameters most influenced the predictions [11].

2.4 Performance evaluation

Model performance was assessed using two standard regressions:

- MAE equation:

$$MAE = \frac{1}{n}\sum |y_i - \hat{y}_i| \tag{6}$$

- RMSE equation:

$$RMSE = \sqrt{\frac{1}{n}\sum (y_i - \hat{y}_i)^2} \tag{7}$$

Where $\hat{y}_i$ is the predicted value.

These features supply insight into the reliability and accuracy of the models. Lower MAE and RMSE values indicate better predictive performance [12].

3 Results and discussion

This research assessed the performance of two ML models–RF and GB–in predicting three key Moldex3D simulation outputs for the polymer material PP Domolen: filling time, packing sprue pressure, and warpage total displacement. The predictions were compared against actual simulation results using MAE and RMSE.

3.1 Prediction accuracy overview

Table 1 summarizes the predicted values from both models alongside the actual Moldex3D simulation results. It also includes the MAE and RMSE metrics for each parameter, allowing a clear comparison of model performance.

Table 1: Comparative performance of RF and GB models against Moldex3D simulation results for PP Domolen

Parameter	RF prediction	GB prediction	Actual value	RF MAE	RF RMSE	GB MAE	GB RMSE
Actual filling time (sec)	2.05165	2.103853248	1.901	0.15065	0.15065	0.202853248	0.202853248
Packing XY sprue pressure (MPa)	127.155	135.2898524	123.746	3.409	3.409	11.54385244	11.54385244
Warpage total displacement (mm)	1.1291	0.797434134	0.035	1.0941	1.0941	0.762434134	0.762434134

3.2 Model performance analysis

To better understand how each model performed across different simulation outputs, we analyze the prediction errors for each parameter individually. This helps identify which model is more suitable for specific types of outputs.

Filling time: Both models produced close predictions, with RF slightly outperforming GB (MAE of 0.151 vs. 0.203). This suggests that RF is more effective for this relatively stable parameter.

Packing pressure: RF again showed better accuracy (MAE of 3.409), while GB overestimated the value significantly (MAE of 11.544). This indicates that packing pressure may be more sensitive to overfitting or noise in small datasets.

Warpage displacement: GB performed better (MAE of 0.762 vs. 1.094), likely due to its capability to model nonlinear behavior more effectively. Warpage is a complex output influenced by multiple interacting factors, making it well-suited for boosting algorithms.

3.3 Visual comparison

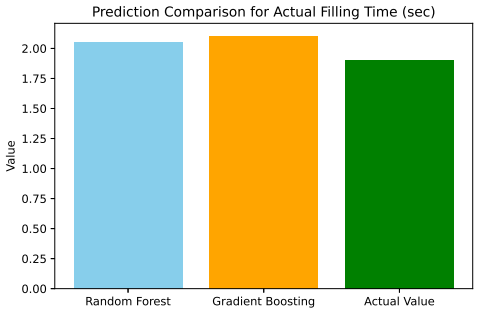
Figure 1 presents a visual comparison of the predicted and actual values for filling time, packing pressure, and warpage. This chart complements the numerical results and highlights the relative accuracy of each model across the three parameters.

3.4 Discussion and implications

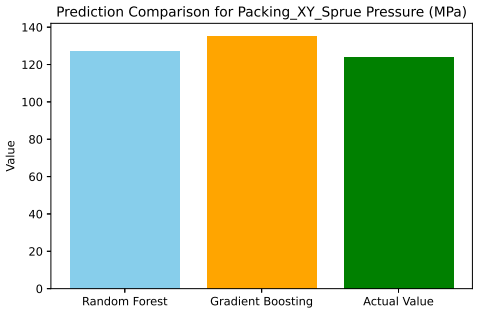
The results demonstrate that machine learning can reliably approximate Moldex3D simulation outputs, offering a faster alternative to full simulations. While RF generally performed better for filling and packing predictions, GB showed strength in modeling warpage.

These findings support the integration of ML into simulation workflows, especially for early-stage design evaluations or material screening. However, the study also highlights the importance of dataset size and diversity–with only two training samples, model generalization is limited. Future work should include:

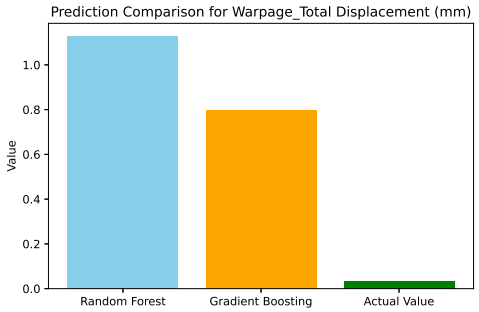
- Expanding the dataset with more materials and process conditions.
- Applying hyperparameter tuning and ensemble stacking.
- Exploring transfer learning for cross-material prediction.



(a) Filling time (sec)



(b) Packing sprue pressure (MPa)



(c) Warpage total displacement (mm)

Figure 1: Prediction vs Moldex3D actual values

4 Conclusion

This paper demonstrated the efficiency of ML to accelerate injection molding simulations by predicting key Moldex3D outputs–filling time, packing sprue pressure, and warpage total displacement–for a third polymer material, PP Domolen, using data from two previously simulated materials. Two ensemble models, RF and GB, were trained on geometric, thermal, and process parameters extracted from Moldex3D. The results proved that:

- RF provided further accurate predictions for filling time and packing pressure, with lower MAE and RMSE values.
- GB outperformed RF in predicting warpage, likely due to its strength in modeling complex, non-linear relationships.
- Both models predicted outcomes that closely matched simulation results, confirming ML's viability as an efficient alternative to full-scale simulations.

The integration of ML into the simulation workflow offers significant advantages, including reduced computational time, faster design iterations, and support for real-time decision-making in polymer process optimization. While this study used a limited dataset, the promising results suggest that expanding the training data and applying advanced techniques like hyperparameter tuning, transfer learning, or model stacking could further enhance prediction accuracy. In future work, we aim to:

- Extend the dataset to include more materials and process conditions.
- Explore deep learning models and hybrid approaches.
- Integrate the ML pipeline into a user-friendly interface for industrial use.

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