Application of machine learning methods for process optimization in electronic packaging processes

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Abstract— Epoxy resins are commonly used as encapsulation materials in electronic packaging processes. Fluctuations in the materials lead to both changes in processability and to varying quality. Ideally, these variations should be identified, and measures taken as quickly as possible to reduce scrap parts and thus costs. A promising optimization approach for encapsulation processes are machine learning models, which have already shown good results in quality predictions, especially for injection molding. Subsequent quality measurements are avoided with good quality prediction models. With this type of models, not only predictions can be made, but also optimal parameter combinations can be found. In this paper, models for predicting quality criteria warpage and residual enthalpy of the epoxy molding compound were set up, trained and validated. Time series of in-situ sensors were used, from which relevant features were extracted and which, together with machine parameters, provide a dataset for prediction. The most promising prediction models are random forest regression and gradient boosting regression. They predict warpage with an accuracy of 90 % to 91 % and the residual enthalpy with an accuracy of 95 %. Subsequently, optimization models of the machine parameters were set up. All relevant target variables were considered in a cost function, through the minimization of which an optimal parameter set was found. The gradient boosted tree and Bayesian optimization were determined to be the most promising models, as they lead to the lowest values of the respective cost function.

Keywords— machine learning methods, warpage prediction, enthalpy prediction, process optimization, molding processes, epoxy molding compounds, electronic packaging

I. Introduction and Motivation

Encapsulation is an essential process step in electronic packaging technology. It involves encapsulating electronics to protect the electronic components from environmental influences, insulate electrical contacts and provide structural support [1]. As encapsulation materials mainly epoxy molding compounds are used in a molding process such as transfer or compression molding [2]. A major problem in this process is batch variation or drifts in material properties, which affects both processability and quality [3]. The quality also depends on the specific process parameters that are selected depending on the material properties of the epoxy resin. Quality criteria for electronic encapsulation are usually warpage, delamination, wire sweep, voids, incomplete filling or curing state of the epoxy molding compound [4].

In recent years, extensive research has been done to achieve a deeper comprehension of these type of processes. For this purpose, various sensors were installed in molding tools to obtain process information during the encapsulation. Classical sensors are temperature and pressure sensors [5], dielectric sensors (DEA) [3][5], ultrasonic sensors [6] or Fourier-transform infrared sensors [7]. For process optimization, mainly simulation models or statistical experimental designs are performed, or adjustments are made purely on empirical data [8]. However, another promising approach is offered by data-driven methods such as machine learning models [9]. They can be used to find underlying structures in data that are not yet perceivable to humans [10].

Machine learning models have already been applied to various plastics processing applications. The most common use case is the injection molding process, where there is already diverse research work on quality prediction or process optimization with machine learning models [11][12]. Tree-based algorithms, regression-based algorithms, or neural networks are applied to perform classifications or regressions [13][14]. An interesting approach is described in [15], where the use of sensor data for prediction models is outlined. The authors identified the cavity pressure as essential for quality, which is why sensor data provide important information. They extracted key features of the recorded time series as additional information for quality predictions. For machine learning models in thermoset processes there is still very few research work. However, there are initial approaches for transfer molding. By applying classification methods, it is possible to predict the filling behavior or voids during transfer molding [9]. Another approach is described in [8] where the authors performed process optimization for transfer molding with neural networks.

In the following, the use of machine learning models for molding processes is presented. First, methods for the prediction of selected quality criteria such as warpage and the residual enthalpy of the molding material are shown. After that, different approaches for the optimization of the process parameters of molding processes are presented.

II. METHODOLOGY

The main objective of this work is the implementation and validation of quality predictive supervised learning models and the optimization of process parameters for molding processes. Therefore, information about data acquisition and the acquired dataset are presented. In addition, the pre-processing of the data and the implemented machine learning models including their evaluation are shown.

A. Data acquisition

In this study, the so-called local pressure molding was used as encapsulation process. This is a combination of conventional transfer molding and compression molding [7][16]. The experiments were carried out with a press from the company Lauffer GmbH & Co. KG (UVKU 125-SO). In this process, a rectangular area with dimensions of 65x35x1 mm is pressed onto a substrate material (200 ı m FR4 R1566, Panasonic Corporation, Kadoma, Japan) in a heated tool. The molding material is a highly filled epoxy molding compound with a filler content of approximately 90 %, which is available in a pre-pressed sheet geometry (Shin-Etsu Chemical Co., Ltd., Tokyo, Japan). A release film (200 ı m single-side matte LM-ETFE film, AGC Chemicals Europe, Ltd., Amsterdam, Netherlands) was used for the experiments. The pressing process is achieved by a piston that compresses the material. During the process, the movement for filling is position-controlled first, which changes to a pressure-controlled profile as soon as the cavity is filled. During the molding process, there are various machine parameters that have an influence on the processability and thus also on the quality of the encapsulation. These are the mold temperature, the cavity pressure, the piston feed speed at which the material is pressed into the cavity, and the cycle time.

To acquire data during the molding process, two temperature sensors T_1 and T_2 (type 6195B, Kistler IInstruments AG, Winterthur, Switzerland), three pressure sensors p_1, p_2 and p_3 (type 6167A, Kistler IInstruments AG, Winterthur, Switzerland) and two dielectric sensors DEA_1 and DEA_2 (4 mm monotrode-sensor 4/3RC, Netzsch-group GmbH & Co. KG, Selb, Germany) were integrated into the molding tool. The sensors are in direct contact with the epoxy molding compound and therefore provide information of the molding material during the process. In addition, the pressure p_4 and the piston position s_1 were also read out directly from the machine. A trigger signal from the machine ensures that the start of the measurements is automated, and the measurements can be correlated with the elapsed process time.

After the encapsulation process, the quality criteria were evaluated, which are the warpage of the pressed parts on the one hand and the residual enthalpy of the epoxy resin on the other. The warpage was evaluated with a 3D profilometer (VR-5000, Keyence AG, Osaka, Japan), obtaining height data. The residual enthalpy of the molding compound was determined by differential scanning calorimetry (DSC 204 F1 Pheonix, Netzsch-Ger±tebau GmbH, Selb, Germany). The residual enthalpy can then be correlated with the curing stage of the molding material.

B. Dataset

In order to obtain an extensive dataset with a large range of different warpage and enthalpy values, the machine parameters were varied. The parameter limits were determined experimentally resulting in the following limits:

- Temperature between 150 éC and 175 éC,
- Pressure between 25 bar and 100 bar,
- Piston feed rate between 0.2 mm/s and 1.0 mm/s and
- Cycle time between 180 s and 900 s.

No statistical experimental design was performed purposefully, as these are often not ideal for machine learning models. Instead, each parameter was varied individually while the others remained constant. A total of 23 parameter combinations were performed with 5 repetitions each. The standard parameter combination at 170 éC, 50 bar, 0.2 mm/s and 300 s was performed more often with 20 replicate trials, resulting in a total dataset size of 135 data points. Warpage and enthalpy were measured and evaluated for each part produced.

C. Data pre-processing

First, features of the time series measured were extracted. Common statistical parameters such as minimum (min), maximum (max) or mean value were calculated as well as additional key features which are all listed in TABLE I. It results in 29 features extracted from the time series in addition to 4 machine parameters.

TABLE I.
FEATURES EXTRACTED FROM THE TIME SERIES

Sensor data	Feature extraction	
	Sensor	Extracted feature
Sensors installed in the tool	T_1, T_2	min, max, mean
	p_1, p_2, p_3	min, max, mean
	DEA_1, DEA_2	min, permittivity at change point (cp), time stamp at change point (ts_cp)
Sensors from machine	p_4	min, max, mean
	s_1	min, max, mean, slope, time stamp at switching point (ts_sp)

After feature extraction, the dataset was split into 60 % training data and 40 % test data. The dataset was grouped so that each experimental combination performed is present at least once in the test data. The subsequent machine learning models are trained using only the training data and finally tested with the test data.

D. Machine learning models

For the prediction of warpage and the residual enthalpy of the molding material different machine learning models were trained. Existing models from the scikit-learn library were applied. Random forest regression, support vector regression, gradient boosting regression and k-nearest neighbors were trained and tested with the previously presented dataset. No hyperparameter optimization was performed as the models were applied with their standard hyperparameters.

The best quality prediction model in each case is required for the following optimization models. The models random search (RS), gradient boosted tree (GBT) and Bayesian optimization (BO) from the scikit-learn library were applied and trained for optimization. The optimization targets were defined as the quality criteria warpage and residual enthalpy. The machine parameters were selected as the parameters to be optimized.

The optimization models are designed to maximize or minimize one target variable. If several variables are to be taken into consideration, they must be combined in a cost function. The optimization models then optimize the cost function by minimization. The definition of a cost function is essential, as it significantly influences the success of the optimization models substantially [17]. All target variables were thus scaled between zero and one. In addition, the scaled quantities can subsequently be weighted depending on the application.

In this study, two different cost functions were implemented and tested. First, the target variables warpage and residual enthalpy were used. The warpage w_{sc} was scaled between 0 μm and 1300 μm since a warpage of 0 μm is targeted and 1300 μm is the maximum occurring warpage. For the enthalpy, a value of 0 J/g, i.e., complete curing, is targeted. The lowest residual enthalpy possible after molding is 8 J/g, so the enthalpy h_{sc} was scaled to these limits. The weights of both quantities w_w and w_h were set to 1 since both target quantities are considered equally important. This results in the cost function described by (1).

$$cost_1 = w_w \cdot w_{sc} + w_h \cdot h_{sc} \tag{1}$$

The second cost function also includes the cycle time t_{sc} in addition to the two target variables. This is limited by the curing of the material and therefore scaled between 60 s and 300 s. The weighting of the cycle time w_t was also set to the value 1, resulting in the cost function shown in formula (2).

$$cost_1 = w_w \cdot w_{sc} + w_h \cdot h_{sc} + w_t \cdot t_{sc} \tag{2}$$

E. Model evaluation

To compare the prediction models, the accuracy of each model was determined by calculating the R^2 value, and the mean absolute error (MAE). In addition, the feature importance was calculated to identify the most relevant features for prediction. Then, the plot of predicted over real values was considered in more detail for the model with the highest accuracy.

For the optimization models, the predicted process parameters and the value of the respective cost function were compared with each other. In addition, the training history is plotted and evaluated for all optimization models presented.

III. RESULTS AND DISCUSSION

Warpage and enthalpy prediction models were trained and tested with the acquired dataset. Different models were evaluated and compared with each other. Subsequently, the most promising predictive models were used for optimization models, which were tested and compared with two different cost functions.

A. Warpage prediction model

The first prediction model is implemented for the quality criterion warpage. The accuracy results and the calculated MAE are shown in TABLE II. The prediction was first performed only with the machine parameters (MP) and then including the extracted features from the sensor timeseries (ts-features).

The warpage predictions with random forest regression and gradient boosting regression show an accuracy of 86 % and an MAE of 36 μm when the prediction was made with machine parameters alone. With a prediction value of 87 %, the model k-nearest neighbors is almost equally as accurate but has a larger MAE. The support vector regression however predicts warpage with an accuracy of 48 %. This is the lowest prediction value, and it causes an MAE of 88 μm. Since the measurement device for warpage measurements exhibits an error up to 10 μm, the prediction with an error of 36 μm to 46 μm is concluded to be satisfying.

TABLE II.
COMPARISON OF DIFFERENT WARPAGE PREDICTION MODELS

Model	Evaluation test data (MP)		Evaluation test data (MP and ts-features)	
	Accuracy (R^2)	MAE	Accuracy (R^2)	MAE
Random forest regression	86 %	36 μm	90 %	45 μm
Support vector regression	48 %	88 μm	72 %	67 μm
Gradient Boosting regression	86 %	36 μm	91 %	38 μm
K-nearest neighbors	87 %	46 μm	86 %	53 μm

Warpage is a very sensitive parameter which, despite supposedly constant machine parameters, shows fluctuations in the warpage measurements. Process deviations for example in the temperature are very common. Despite the same temperature set in the machine, the parts are produced with different temperatures which is why in-situ measurements are necessary and provide important information. Therefore, warpage prediction was performed with machine parameters and extracted features from sensor data. Whereas the prediction accuracy with the model k-nearest neighbors is almost the same for both datasets, all the other models show improvements in their prediction accuracy. Random forest regression and gradient boosting regression show an accuracy of 90 % respectively 91 %. The accuracy with support vector regression is even improved by 24 % to an accuracy of 72 %. The improvement in the prediction accuracies is reasoned to be due to the additional information provided by the extracted features. There is however a risk of overfitting the models since the dataset has only 135 samples. Overfitting can be avoided by adding more samples to the dataset or by hyperparameter optimization of the prediction models (e.g., early stopping).

To identify the most relevant features for the prediction of warpage the feature importances are plotted in Fig. 1. The most important feature for random forest regression, gradient boosting regression and k-nearest neighbors is by far the cycle time. For random forest regression besides the cycle time, DEA_2_min is considered as an important feature whereas the importance is factor 7 lower compared to the cycle time. The gradient boosting regression model considers T_2_max as the second important feature and k-nearest neighbor DEA_ts_cp with a factor of 4 and 10 less importance compared to cycle time, respectively. In the dataset it is visible, that long cycle times lead to low warpage values which is why the cycle time is considered as the most important feature.

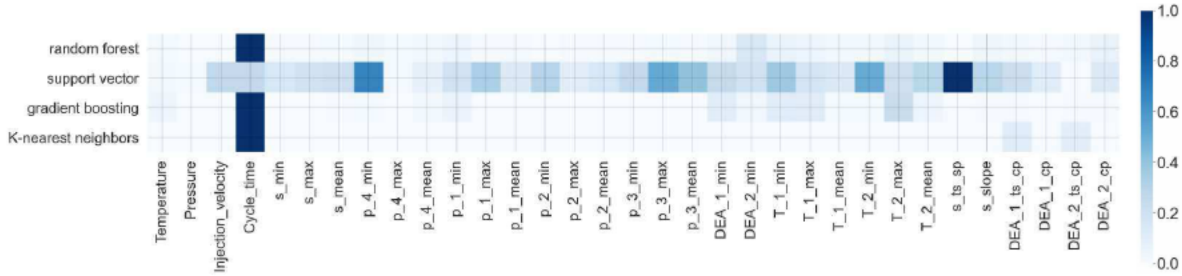

Fig. 1 Feature importance of warpage prediction models

The feature importance of the support vector regression model is different compared to the other models. Multiple features are considered as important whereas the features s_ts_sp and p_4_min are of utmost importance. Apparently, the support vector regression model does not correctly recognize the significant correlations in the dataset, which is why the prediction values for this model are lower than for the other models tested.

Features extracted from time series in addition to the machine parameters are helpful to identify outliers since warpage prediction accuracy scores are higher when features of time series are included. However, Fig. 1 shows that the cycle time is the most important feature for warpage prediction. This is why the prediction accuracies are hardly lower when only machine parameters are used for prediction.

In Fig. 2 the predicted against the real warpage values of the test data for random forest regression is shown since this model exhibits a high accuracy at 90 %. It is clear that the predicted warpage values are close to the real warpage values, indicating an accurate prediction model. The model could be improved by extending the dataset since there are only a few datapoints above 900 µm.

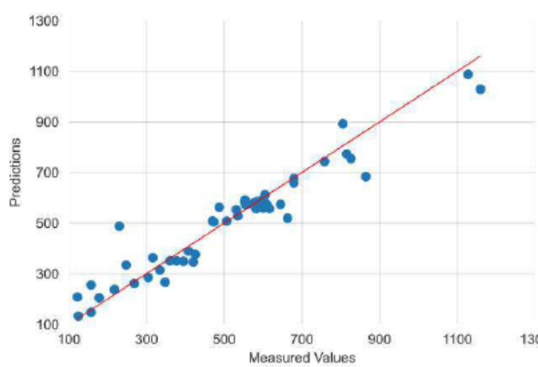

Fig. 2. Comparison of predicted and real warpage values for random forest regression

B. Enthalpy prediction model

The second prediction model is implemented for the quality criterion enthalpy. TABLE III. shows the accuracy results and the calculated MAE for the prediction with machine parameters and after sensor timeseries are included. The enthalpy prediction with random forest regression and gradient boosting regression displays an accuracy of 95 % when the prediction is made with machine parameters. The accuracy values do not change when the features are applied for prediction. This leads to an MAE of 0.15 J/g. The model k-nearest neighbors predicts the residual enthalpy with an accuracy of 85 % when machine parameters are applied, and 96 % when the features from the sensor timeseries are included for prediction. The model support vector regression is not able to predict any reasonable prediction values. It is concluded that this model fails for enthalpy prediction.

TABLE III.
COMPARISON OF DIFFERENT ENTHALPY PREDICTION MODELS

Model	Evaluation test data (MP)		Evaluation test data (MP and ts-features)	
	Accuracy (R^2)	MAE	Accuracy (R^2)	MAE
Random forest regression	95 %	0.15 J/g	95 %	0.15 J/g
Support vector regression	-	-	-	-
Gradient Boosting regression	95 %	0.13 J/g	95 %	0.12 J/g
K-nearest neighbors	85 %	0.24 J/g	96 %	0.12 J/g

The residual enthalpy is determined based on DSC measurements of the produced parts. On the material side, the minimum cycle time is limited to 180 s, which corresponds to a maximum residual enthalpy of 8 J/g. Even with a slight increase in the cycle time, the residual enthalpy drops to values close to 0 J/g, which corresponds to complete curing. Therefore, the dataset contains mainly enthalpy values close to 0 J/g. Since the measurement device for enthalpy measurements exhibits an error up to 2 J/g, the prediction with an error below 1 J/g is concluded to be satisfying. It is concluded that prediction with accuracies of more than 85 % are very accurate.

Fig. 3. shows the importance of the individual features for the prediction of the residual enthalpy. It is clear, that the most important feature is the cycle time, when random forest regression, gradient boosting regression or k-nearest neighbors is applied. For k-nearest neighbors the feature DEA_2_ts_cp is considered as relevant with the importance being by factor 20 lower compared to the cycle time. This is the reason why the prediction accuracy improves by 11 % when the features are applied for prediction. The model support vector regression considers multiple features as important but since the prediction for residual enthalpy fails it is not considered further.

Another approach which is not presented in this work, is the prediction of the residual enthalpy with spectral data. Regression models can be trained on the change of infrared spectra, since the spectra change with increasing curing of the

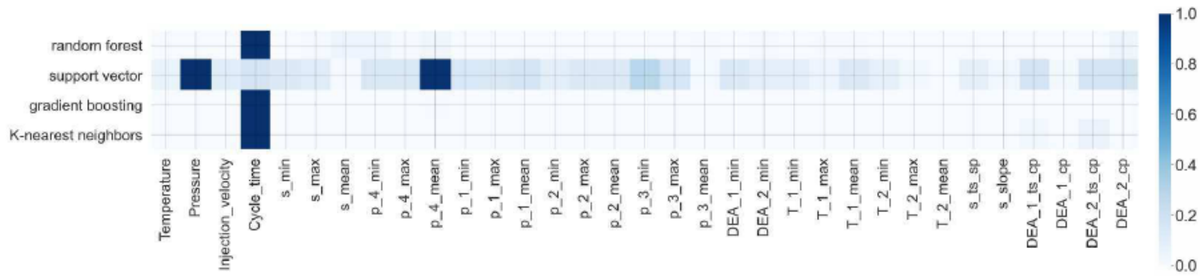

Fig. 3 Feature importance of enthalpy prediction models

material. The changes in spectra can be correlated with the residual enthalpy. This approach has been proven several times in literature [18] and could lead to better prediction results.

C. Optimization approach

First, cost function (1) is minimized with the presented optimization models. For these models a prediction model for each quality criteria needs to be defined. The prediction models are trained on the presented dataset and then applied for the parameter combinations, that the optimization models suggest during optimization. The random forest regression model was chosen as a prediction model for warpage and enthalpy since it performed well for both quality criteria. The prediction models were trained on machine parameters only.

TABLE IV displays the optimized results for random search, Bayesian optimization and gradient boosted trees. The three optimization models predict similar optimized process parameters. Cycle time and temperature are the two decisive factors regarding warpage and enthalpy whereas the cavity pressure and injection velocity have no noticeable influence on the two quality criteria. All optimization models predict long cycle times which is clear since the cycle time is not considered in cost function (1) and long cycle times lead to low warpage values. The model gradient boosted trees reaches the lowest value of the cost function. The optimized process parameters lead to a predicted warpage value of 121 μm and a predicted enthalpy value of 0.0 J/g which are reasonable predictions.

TABLE IV.
OPTIMIZED PROCESS PARAMETERS WITH COSTFUNCTION (1)

Model	Predicted process parameters				Optimized value cost function
	T	p	t	v	
RS	159°C	54 bar	838 s	0.2 mm/s	0.0944
BO	158 °C	100 bar	832 s	0.2 mm/s	0.0938
GBT	159 °C	64 bar	824 s	0.3 mm/s	0.0635

To compare the models with each other, a convergence plot of the three models was created in Fig. 4 by visualizing the value of the cost function against the number of iterations. It is clear, that all models achieve an optimization of the cost function after a few iteration steps. The lowest value is achieved with gradient boosted trees after 28 iteration steps. The success of these optimization models depends on several factors. One factor, is the setup of the cost function, for which there are unlimited possibilities. Additional process knowledge is required, such as for the scaling of the variables to be optimized. Furthermore, the weights can be varied, which also influence the result of the optimization.

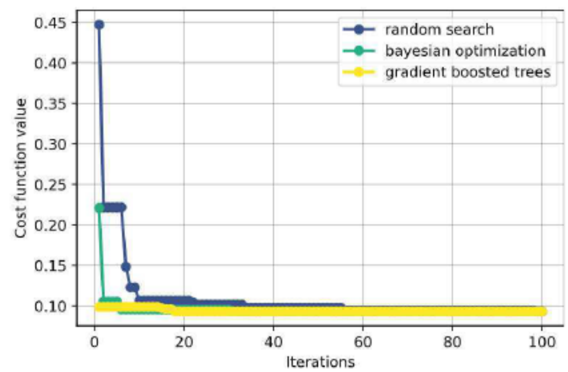

Fig. 4. Development of cost function 1 against iteration steps

For consideration of the cycle time, the optimization models were applied to cost function (2). The optimized process parameters are presented in TABLE V. The models behave similarly to cost function (1) with the Bayesian optimization achieving the lowest value of the cost function. Bayesian optimization predicts a cycle time of 396 s compared to 832 s when cost function (1) was considered. This is a reduction of 52.4 % in cycle time. The optimized process parameters lead to a predicted warpage of 180 μm and a predicted residual enthalpy of 0.0 J/g. The predicted warpage increases compared to cost function (1) because cycle time was added in cost function (2).

TABLE V.
OPTIMIZED PROCESS PARAMETERS WITH COSTFUNCTION (2)

Model	Predicted process parameters				Optimized value cost function
	T	p	t	v	
RS	160 °C	86 bar	404s	0.2 mm/s	0.4496
BO	162 °C	39 bar	396 s	1.0 mm/s	0.4412
GBT	158 °C	29 bar	421 s	0.2 mm/s	0.4537

Fig. 5 shows the convergence plot of all models for the optimization of cost function (2). All models achieve minimization in the cost function after a few iteration steps whereas the decrease in cost function (2) is visible after more iteration steps compared to cost function (1). The lowest value in cost function is achieved by Bayesian optimization after 25 iteration steps indicating the most promising optimization method for cost function (2).

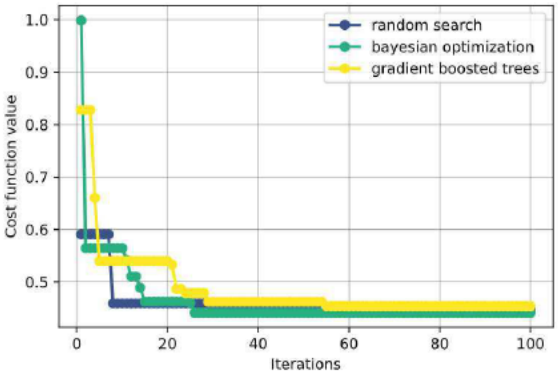

Fig. 5. Development of cost function 2 against iteration steps

IV. CONCLUSION AND OUTLOOK

The models presented in this work allow accurate quality predictions for warpage and residual enthalpy. Several prediction models were tested and compared, with gradient boosting regression and random forest regression achieving promising predictions for both quality criteria. It is possible to test other models such as neural networks in order to make better predictions. Also, it is possible to expand the dataset for better prediction, as many machine learning models tend to perform better on large datasets. The prediction of warpage with the use of machine parameters and sensor data appears to be useful and promising.

In addition, different optimization models were implemented and validated to find the optimized process parameters. All relevant criteria were considered in a cost function. The best optimization model is found in the gradient boosted trees model for cost function (1), and in Bayesian optimization for cost function (2). These models achieve the lowest value for each cost function and predict reasonable process parameters. A disadvantage of the presented models is that they are necessarily not able to predict values outside their data range. For future optimizations it is also possible to use another kind of models like reinforcement learning models. These models do not need a large dataset at the beginning, but learn continuously. This could be a completely new approach for optimization of molding processes.

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