Quicker Evaluation of the Optimum Operating Point

Machine Learning: Combining Simulation and Experimental Test Data

The resource-economical determination of an optimized operating point in injection molding is still a challenge. Machine learning offers great potential for re-using knowledge from a flow simulation that has already been generated. By transferring methods for combining simulation and experimental test data, the testing effort during sampling can be reduced significantly.

Significant reduction of the effort for determining the optimum operating point by machine learning © Christin Gerstner / Julia Volke

Flow simulations are used to design injection molds in order to model mold filling and identify possible critical quality deficiencies at an early stage [1]. In the subsequent step of defining the operating point as part of sampling, simulations only play a minor role. This is because the simulation quality varies in dependence on the setting parameters [2, 3] and is therefore difficult to determine. In order to be able to use simulations for sampling, it is necessary to assess the simulation quality. Based on this assessment, simulations can be used effectively for reducing the experimental test effort in order to determine an optimized operating point. The Department of Plastics Technology in the Institute of Materials Engineering (IfW) at the University of Kassel, Germany, in cooperation with the working group on Virtual Machining (VM) at the chair of software engineering at the Technical University of Dortmund, Germany, has developed models for calculating the part properties by combining the use of simulation and experimental data. The goal of this is a successful data-driven determination of the operating point by applying machine learning methods.

Predicting the Simulation Quality to Reduce the Test Effort

The practical determination of the process setting can be performed based on various strategies during sampling [4–6], and usually depends on the experience of the machine operator. Irrespective of the chosen strategy, the focus is on determining an operating point with which the required part properties can be achieved. Some suppliers, such as Arburg, Engel and Wittmann Battenfeld already offer the operator the possibility to visualize the results of the flow simulations performed on the machine, and thus obtaining information about the filling behavior [7]. Direct information about the optimum operating point cannot be obtained yet.

In the research, data-driven modeling of the relationships between setting parameters and part properties based on simulation data [8–14] or experimental data [15–22] has already been widely investigated. Modeling based on both data sources offers great potential [2, 3] and is currently supported by two trends: first, the increasing computational capacities for generating simulation data and second, the growing number of possibilities for in-process data acquisition in injection molding processes.

In order to assess which simulation can replace an experiment, an evaluation of the simulation quality must be performed. The prediction of the simulation quality as well as the part quality can be predicted on the basis of different methods of machine learning, whose transfer to a practice-oriented application with experimental data from real processes is currently still a challenge [23]. One reason for this is the heterogeneous data structures of the simulation and test data.

As part of the cooperation between the IfW and the VM working group, the simulation data and experimental data were compared, in order to subsequently determine an operating point

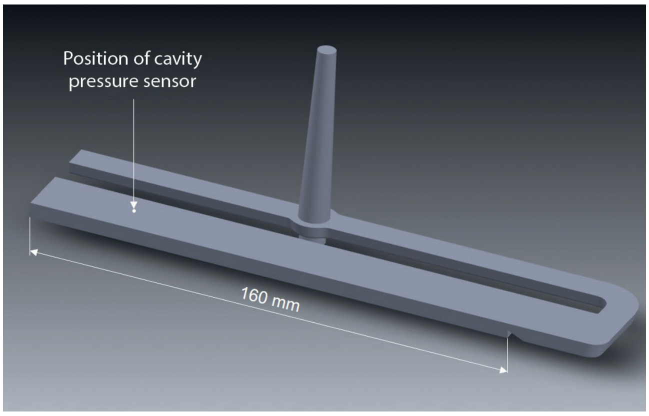

Fig. 1. This flat bar was used for determining the real and simulated part properties © IfW

with as little experimental effort as possible. By creating the models for different part variants, the knowledge generated in the models can be transferred to other parts. For this purpose, a mold was used in which the part thickness was varied using four different mold inserts. The data of three mold inserts were used to train the models, which were subsequently tested with data from a fourth mold insert. Among other results, the prediction quality of different machine learning methods was assessed.

Generating a Suitable Database

The basis for a successful model generation is a suitable database. Both experiments and simulations were therefore performed based on a stochastic test design. In order to obtain the maximum information about the process with minimum experimental effort, a combined test design was prepared, comprising the methods of a latin hypercube test design [24] and a full-factorial test design. Latin-hypercube test designs allow uniform coverage of the multidimensional factor space with reduced test effort [25]. The test points are distributed randomly and uniformly in the parameter space [26]. However, strongly varying factor settings are not practicable in injection molding because of the thermal inertia and the start-

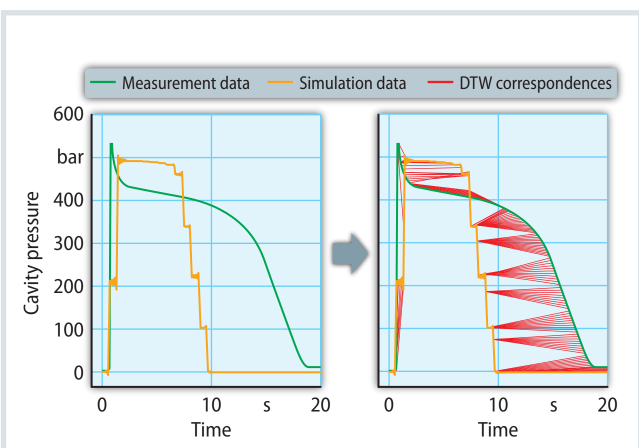

Fig. 2. Measured and simulated profile of the cavity pressure and computation of the DTW correspondences [27] Source: IfW and VM; graphic © Hanser

Setting parameters test design	Process data profiles	Quality features
Injection flow rate [cm³/s]	Injection pressure [bar]	Thickness, 4 measurement points [mm]
Holding pressure level [bar]	Injection flow rate [cm³/s]	Weight [g]
Cylinder temperatures [°C]	Cavity pressure [bar]	
Mold temperature [°C]	Volumetric filling of the cavity/screw volume [%]	

Table 1. Test design parameters, process data profiles and quality features for generating a suitable database Source: IfW

up behavior. Therefore the parameters of the heating zone temperatures in the plasticizing unit, as well as the mold temperature were varied only between two fixed factor steps. The injection flow rate as well as the holding pressure level were determined within predefined parameter limits according to the latin-hypercube scheme.

For all the test configurations, various process data were recorded, and quality features were determined (**Table 1**). The setting parameters from the experimental design were used for parameterizing the simulation and the injection molding process. The process provides data that are recorded on the injection molding machine and are computed in the simulation as time series.

For further modeling, the complete time series of the process data were used, because characteristic values, such as the minimum, maximum or integral values, would result in an information loss. The properties of the parts are quantified via the quality features thickness and weight.

The basic prerequisite for a comparison is the equivalent representation of the factors, process data and quality features as well as the quantifying of these parameters in the simulation and in the injection molding process.

Comparison between Simulation Results and Experimental Data

The simulations were performed with the software Moldflow Insight 2019.0.5 (Autodesk) and the time series of the computed process data were exported. The experimental process data were exported via the control system of the injection molding machine used (type: Allrounder 320 C Golden Edition, manufacturer: Arburg). The investigated part is a flat bar with a length of 160 mm (**Fig. 1**). The thickness of the flat bar was varied between 2 and 5 mm by means of four different mold inserts. To test the transfer of the trained models to unseen parts, the models were trained with data from three part thicknesses and were subsequently tested with the data from a fourth part thickness.

In order to be able to quantify how well a simulation model represents a real experiment, the data profiles of the injection flow rate, the cavity pressure, the volumetric cavity filling as well as the screw volume, which were simulated and recorded in the experiment, are compared using dynamic time warping (DTW) correspondences. The DTW algorithm can be used to compare the process data profiles despite a very heterogeneous data structure (**Fig. 2**). This comparison is required to compute similar-

Thickness [mm]	Max. cylinder temperature [°C]	Mold temperature [°C]	Injection flow rate [cm³]	Holding pressure [bar]	Similarity [%]
4	270	50	49	496	98.6431
4	250	80	49	496	98.5992
2	270	80	23	406	98.5638
5	250	50	33	443	98.5402

Table 2. Process settings in which the highest similarity between the simulation and experimental data were determined [27] Source: IfW / VM

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German Version

- Read the German version of the article in our magazine *Kunststoffe* or at *www.kunststoffe.de* ities in the following step. The similarity describes how well the simulated data matches the experimental data. For calculating the similarity, the mean value from the normalized DTW correspondences of all process data and the normalized absolute deviations of the measured and simulated quality features were computed. A high value of the computed similarity indicates a strong similarity between the simulation and actual experiment.

To be able to make a statement about for which experimental configurations a simulation serves as a substitution for an experiment and about which parameter values make an experiment mandatory, an ML model was trained, which models the relationship between the setting parameters and the computed similarities. In the case of high predicted similarities, the simulations can be used to replace an experiment (**Table 2**).

Prediction of the Part Properties for Determining the Operating Point

The suitable database and the resulting similarity analysis and prediction were used to train another model, which uses the combined data sources to predict the quality of the injection-molded part in dependence on the setting parameters of the machine (**Fig. 3**). The models for predicting the similarities and the quality were trained using the following methods:

- Linear regression with regularization methods (ridge, Lasso, elastic net),
- random forest,
- adaptive boosting,
- gradient boosting,
- extreme gradient boosting.

To assess the quality of the methods, the root mean square error (RMSE) is used. The computed values of the predicted weight and the part thickness, represented in dependence on the proportion of the used simulation data, show very good results (**Fig. 4**) [27]. For the computed values of the part thickness, the elbow of the curve [28] can be determined to identify an optimum point that models a suitable compromise between the amount of simulation data and the prediction error. Correspondingly, the experimental effort can be reduced by about 62% with minor losses in the prediction quality.

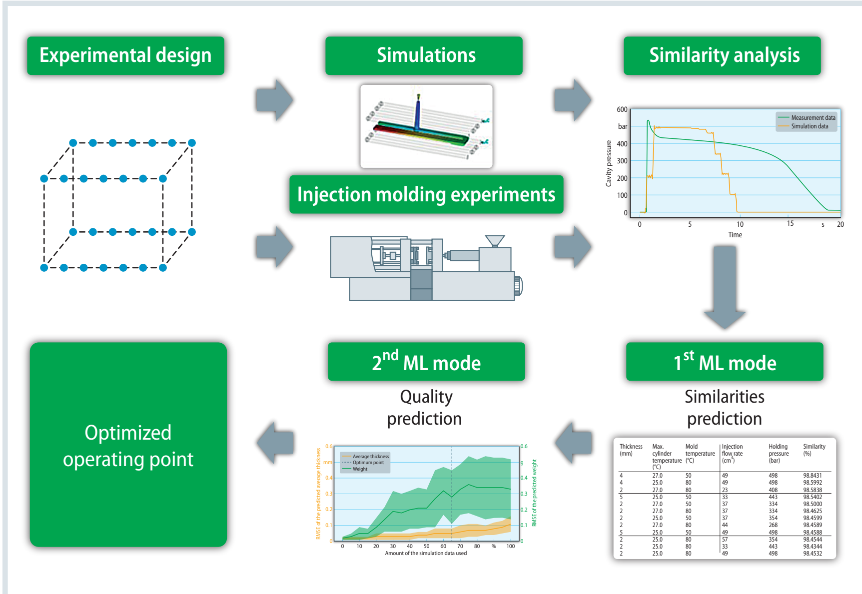

Fig. 3. Concept of the ML models for data-driven determination of the optimum operating point Source: IfW; graphic: © Hanser

Outlook

By using DTW correspondences to compare simulation and experimental data and computing the similarities, a successful method for assessing the simulation quality was developed. The presented models enable the usage ot the generated knowledge in the flow simulation to reduce the necessary experimental test effort for determining the part properties in dependence on the setting parameters on the machine. The high accuracies for prediction of the part properties show that the models based on simulation and experimental data are useful in practice. The principle transferability of the models to unseen parts has already been demonstrated by the fact that it can be transferred to different part thicknesses [27].

For further validation, the methods are adapted to more complex molds in the next step. Through transfer of the generated knowledge to unseen parts and continuous extension of the database, it is ensured that the models can be used in practice. As a result, it will be possible in the future to make property predictions as part of sampling with considerably reduced expenditure of resources. An objective of future studies will be to assess the quality of the transferability to unseen parts depending on the part complexity. ■

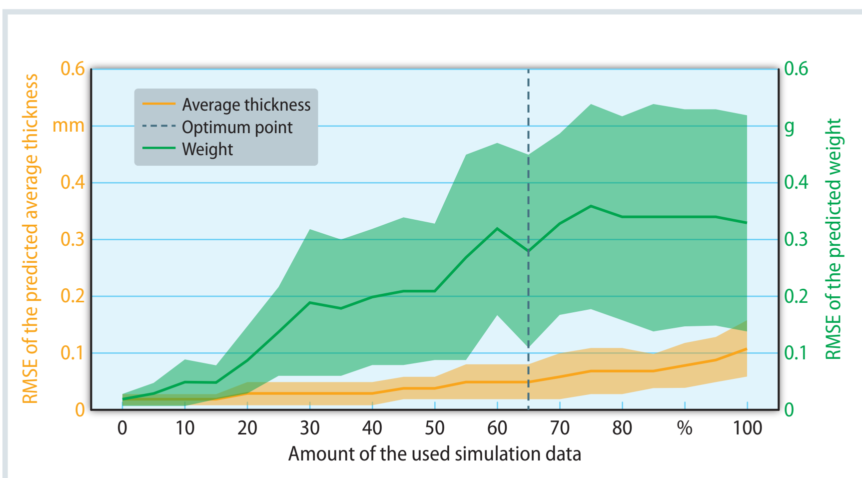

Fig. 4. Results for prediction of the part thickness and weight, shown in dependence on the proportion of the used simulation [27]; RMSE: root mean square error Source: VM; graphic: © Hanser