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D. Biermann, S. Hess, A. Ries, T. Wagner, and A. Wibbeke

Optimization of Thermomechanical Processes for the Functional Gradation of Polymers by Means of Advanced Empirical Modeling Techniques

D. Biermann[1], S. Hess[1]*, A. Ries[2], T.Wagner[1] and A. Wibbeke[3]

[1]*Institute of Machining Technology, Technische Universität Dortmund, Germany – biermann@isf.de; hess@isf.de; wagner@isf.de*
[2]*Institute of Materials Engineering, University of Kassel, Germany – angela.ries@uni-kassel.de*
[3]*Polymer Engineering Paderborn, University of Paderborn, Germany – andrea.wibbeke@ktp.upb.de*

Abstract
I In this paper, an optimization procedure for complex manufacturing processes is presented. The procedure is based on advanced empirical modeling techniques and will be presented in two parts. The first part comprises the selection and generation of the empirical surrogate models. The process organization and the design of experiments are taken into account. In order to analyze and optimize the processes based on the empirical models, advanced methods and tools are presented in the second part. These tools include visualization methods and a sensitivity and robustness analysis. Moreover, the obtained surrogate models are used for a model-based multi-objective optimization in order to explore the gradation potential of the processes. The procedure is applied to two thermo-mechanical processes for the functional gradation of polymers – a monoxiale stretching of polycarbonate films and a compression moulding process for polypropylene sheets.

Keywords: Functionally graded materials, empirical modeling, design and analysis of computer experiments, multi-objective optimization, polymers

INTRODUCTION

The functional gradation of components by means of complex thermomechanical manufacturing processes provides new potentials for the product designer. In order to efficiently check the producibility of a component and to optimize the parameters of the process chain with respect to the specification, novel methods for the modeling and optimization of manufacturing process chains have to be developed. In this context, the major challenge is the generation of precise empirical surrogate models within a strictly limited number of real-world experiments, as standard polynomial regression models are often unsuitable to describe the nonlinear functional relationship between the parameters and the distribution of the component properties.

In this paper, powerful and flexible modeling techniques from the design and analysis of computer experiments (DACE) are therefore enhanced to cope with noisy real-world measurement data. The suitability of these models is demonstrated based on two exemplary processes for the thermomechanical gradation of polymers – a monoxiale stretching of polycarbonate films and a combined heating and compression moulding of polypropylene laminates. Components properties, such as tensile strength, Young's elastic modulus, and damping are predicted over the range of process parameters. Based on the hot compaction process subsequent to a differential preheating, also the description of process chains by means of the surrogate models is presented. In this case, the material temperature acts as a technological interface between the models for each process step. By applying methods of functional analysis of variance, the influence of these interfaces and the process parameters on the graded properties can be quantified. Along with the information about the variations in these interfaces, the robustness of the process chain can be optimized.

The surrogate models establish the basis for the optimization of process parameters with respect to a given specification. In order to restrict the optimization to appropriate process chains, however, the potential for a gradation provided by a specific process chain should be evaluated prior to the actual planning. To accomplish this, a multi-objective optimization of the component properties predicted by the models allows the tradeoffs that can be realized to be assessed. Thereby, the additional estimation of the uncertainty in the component properties inherent in the DACE models can be utilized for sequentially refining the models in order to locally improve the prediction quality in the area of the optimal tradeoff solutions.

OPTIMIZATION PROCEDURE

Empirical Modeling

The optimization of the process chain is conceptually divided into two parts. Fig. 1 shows the respective phases and milestones diagram. At first, the relevant process parameters (input variables) and the output variables (objectives, process responses) are identified.

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To accomplish this, the design space of all possible input parameter configurations, needs to be restricted through screening, experience or prior knowledge about the process. The second step involves the generation of a design of experiments (DOE). Common DOE methods like central composite designs often have some major drawbacks since they restrict the analysis to ordinary polynomial regression models. These models may be useful for processes with linear or quadratic relationship between input parameters and objectives, but they show a poor prediction quality in case of highly non-linear problems [1]. Space-filling designs like Latin Hypercube Designs [2], however, are a recommended choice since they provide a flexible basis for the surrogate model selection.

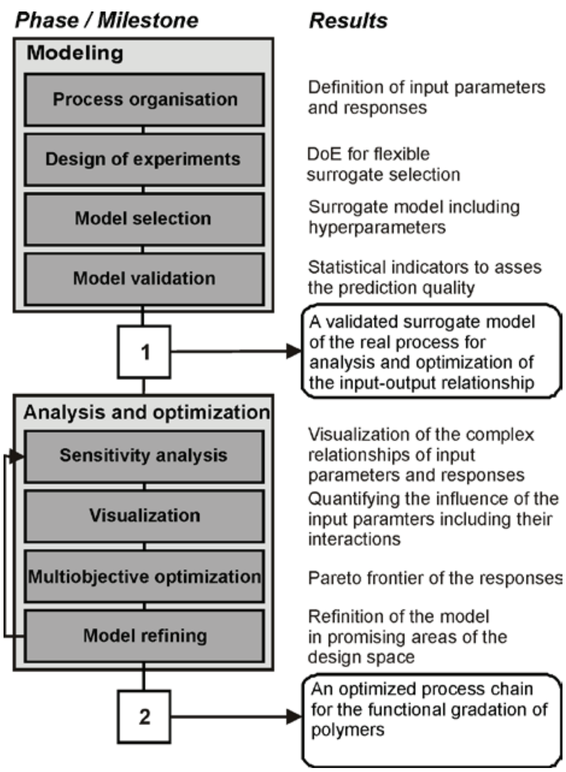

FIGURE 1 – Phases and milestones diagram for the optimization procedure.

This model selection is a challenging part due to the large number of modern statistical learning techniques [3]. Prior research figured out that DACE models often show a very good fit and prediction quality for estimating functionally graded properties [4], [5]. Another advantage is that they provide local uncertainty estimates. This allows the model to be refinement in the respective regions of the design space. If the design of experiments can take place in a sequential manner, the model selection can also be performed by means ensemble techniques [6].
To verify the fitness and the prediction quality of the model, a model validation has to be performed. Therefore validation techniques like residual analysis, bootstrapping or cross validation are used [7]. These methods provide reliable indicators, whether the model selection has to be questioned or whether the selected model precisely describes the considered process.

Analysis and Optimization
The surrogate models provide an excellent basis for analysis and optimization. In a first step, the influence of the different input parameters is investigated. This is done through a sensitivity analysis. Based on the surrogate model, the influenced of the input parameters on the response behavior is analyzed. One possible approach to quantify the proportion of influence is the functional analysis of variance (FANOVA) [8]. The regression function of the surrogate model is systematically divided into single parameter effects or interactions of two or more parameters. Hence, it is possible to calculate the proportion of variance of each parameter and to quantify its impact on the objective. This information can also be visualized in the next step. With the knowledge of the parameters having a particularly high impact, the analysis can focus on the interaction between these parameters and the response. The visualization of surrogate models can be carried out by 2D or 3D plots. The goal of this step is to visualize the complex relationships as clear and intuitive as possible.
Furthermore, the models can be used for optimization. In general, however, not only one objective, but a set of objectives needs to be considered. Since these objectives are often contradictory, it is not possible to obtain one single optimum solution. Rather, the goal is to find a whole set of optimal solutions, the so called Pareto frontier. This set consists of all Pareto-optimal points of the design space, which means that an objective cannot be improved without worsening another. By multi-objective optimization algorithms, it is possible to approximate the Pareto frontier of the process step which allows the potentials of the process to be evaluated.

RESULTS AND DISCUSSION

In this section, the optimization procedure is exemplarily applied to two processes for functional gradation of polymers. The first process is a stretching of polycarbonate films made of Makrolon 2805 from the company Bayer Material Science AG. Makrolon 2805 exhibits a moderate molecular weight and is a non-reinforced type for injection molding. The glass transition temperature is 145 °C and MFR is 10 g/10 min. The MFR is measured according to the testing standard DIN EN ISO 1133 using 1.2 kg polycarbonate at 300 °C [9]. Using a single screw extruder made by the company Battenfeld (Uni Ex 1-45-24/30), the polycarbonate was plasticated using a L/D ratio of 30 and barrel temperatures from 240 °C to 280 °C together with a screw rotation speed of 45 rpm. The subsequent molding was carried out using a wide fishtail nozzle and a gap width of 0.5 mm at 280 °C.

The molding was released and smoothed by means of Dr. Collin's chill-rolling equipment applied at 4.5 m/min and a temperature of 50 °C. Following this, the polycarbonate film was stretched by in the narrow gap on the uniaxial stretching equipment MDO A / MDO B from Dr. Collin. The stretching equipment consists of two roller units. The stretch gap length is given as s = 32 mm [10]. The monoxiale stretching of polycarbonate film causes the macromolecules to become orientated. Previous investigations to the stretching of polycarbonate film have shown that an increase in the strength and Young's modulus is produced [11,12,13]. The input parameters are rotation speed v_1 of roll unit 1 (0.5 m/min to 2m/min), the stretching ratio R_S between both roll units (1 to 4), the annealing temperature T_A (90°C to 140°C) and the stretching temperature T_S (150°C to 160°C). The design of experiments was created by means of a Latin Hypercube sampling with 20 observations.

The other process used for self-reinforced polypropylene composites is compression moulding [14]. For this purpose, 16 layers of mono-extruded twill weave manufactured by the company Bonar, Belgium, are fixated in a tenter frame and pre-tempered in a IR preheating sequence. In order to specifically enhance the thermal influence on the later composite properties, half of the heating panel is covered with a masking sheet to keep the tape fabric located beneath it at a low preheating temperature. After an automatic transfer of the tenter frame into a pressing unit, the compression moulding process is then carried out and incorporates a thermo-mechanical gradation process. The tool especially designed for this process enables a setting of differing press temperatures, so as to be able to complete the thermal gradation on the right and left halves of the tool. This differential tempering is analogous to that carried out in the preheating station. Furthermore, the pressing tool has a triangular shaped geometry, which, due to its special geometry, induces a pressure reduction of 30% on the slants of the triangle in comparison to the other tool areas. Thus, it is possible to create 4 different gradation zones at the same time which result from the differing temperature (right and left) and press force (flat areas, slants) settings [15]. The input parameters are pressure (1Mpa to 3Mpa), the pressing temperature T_A (150°C to 200°C), the pressing time (10s to 180s) and the material temperature T_m as output of the preceding preheating process (24°C to 130°C). The design of experiments was also created by means of a Latin Hypercube sampling. 25 experiments in 5 different zones were performed and therefore 125 observations could be used for empirical modeling.

Based on the surrogate models, a sensitivity analysis can be performed. Via a FANOVA-decomposition, the influence of each input parameter on the response can be quantified. Fig. 2 shows the result for the stretching process with Young's modulus as response. It can be seen that the results for Young's modulus are almost completely described by the stretching ratio and its interaction with the stretching speed. The annealing temperature and the stretching temperature cannot be considered to have a significant influence.

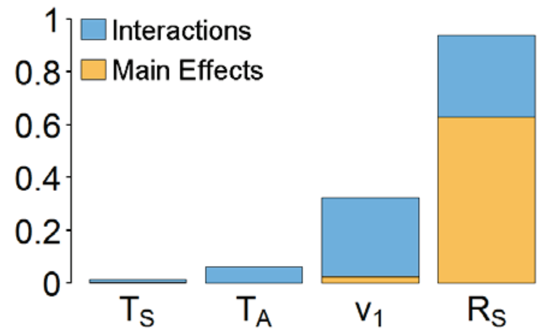

FIGURE 2 – Barplot of the proportion of influence on Young's modulus.

Therefore, Fig. 3 visualizes the influence of stretching ratio and stretching speed on the response. The best results are obviously reached for a stretching ratio between 2 and 3 and high stretching speed values as well as a high stretching ratio combined with a low stretching speed.

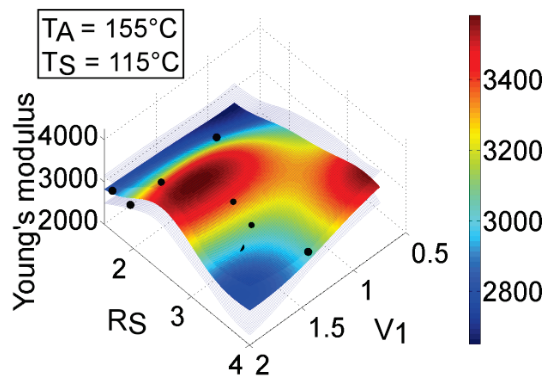

FIGURE 3 – 3D effect plot of the input parameters T_p and T_m on the Young's modulus.

Fig. 4 shows the results for the compression moulding process with the maximum force F_{max} of 10 J impact testing as response. The pressing temperature clearly has the greatest influence on F_{max}. The material temperature and the pressing time are also influential through interactions with the pressing temperature.

Fig. 5 depict, that the interaction of T_M and T_p can mainly be observed at the transitions between the material states otherwise determined by T_p. Therefore, this parameter should not be neglected, since it is also a Technological Interface [16]. This means, it can only be varied in a previous process and is thus expected to have a large variation. Therefore, it should be included in further analyses.

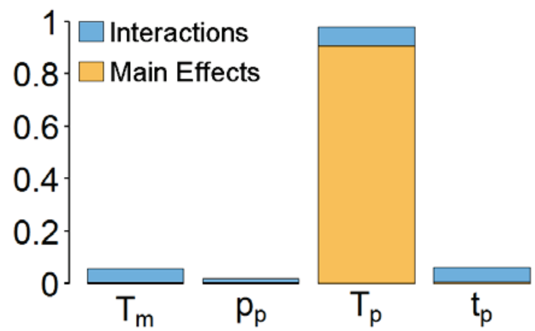

FIGURE 4 – Barplot of the proportion of influence on the response F_{max}.

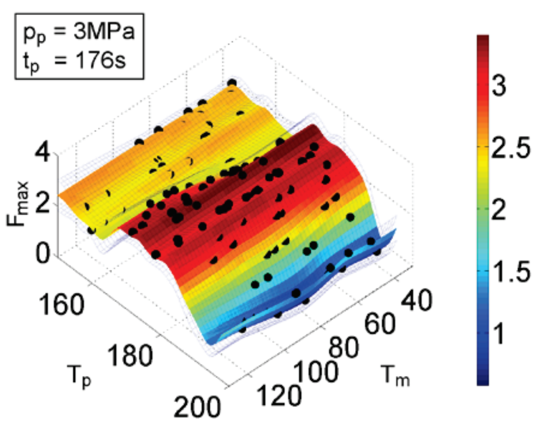

FIGURE 5 – 3D effect plot of the input parameters T_p and T_m on F_{max}.

Since the empirical models provide an efficient surrogate for the actual system, they can also be used for robustness analysis. This can be accomplished, for example, by means of a Monte Carlo simulation. In such a simulation, variations in the input parameters (due to external interference) are simulated and the corresponding behavior of the response is simulated. Fig. 6 exemplarily shows how these uncertainties affect the results for F_{max} in the compression moulding process. It is obvious that a pressing temperature around T_p = 170 °C (yellow) and T_p = 190 °C (purple) leads to a high variation in the output. With these settings, the process cannot be considered as being robust. The simulation shows further, that the best result with respect to robustness and a maximization of the response value is found if the pressing temperature is set to T_p = 180 °C (green). With this setting, a stable consolidation results in a narrow distribution of response values with a mean of 3.25 kN despite of the high variation within the input variables. Also with a pressing temperature of T_p = 160 °C (red) robust results are found, but the mean of the response values is considerably lower (2.45 kN) as a consolidation is never achieved.

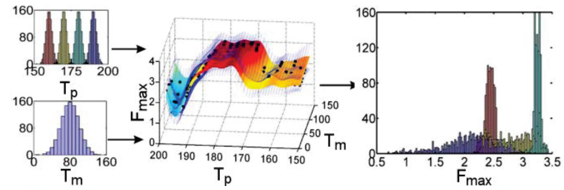

FIGURE 6 – Results of a Monte Carlo simulation with different pressing temperatures. The left histogram shows the simulated distribution of the input parameters T_m, and T_p, and the right side the distribution of the response value F_{max}.

By means of the impact characterization, different material properties can be measured. Hence, the potential of the process can be estimated by means of multi-objective optimization methods. Besides the already discussed F_{max} giving an estimate of the hardness of the component, other objectives like the maximum deformation l_{max} can be used to evaluate its ductility. Fig. 7 shows the approximate Pareto Frontier for both objectives. It can be seen that the two objectives cannot be jointly maximized. A desired l_{max} of more than 11mm, for example, cannot be reached without keeping F_{max} below 3.3 kN. The Pareto Frontier allows these trade-offs to be assessed. It can therefore help, to select the process with respect to the desired specifications.

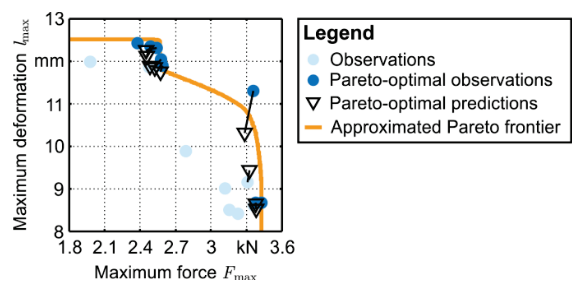

FIGURE 7 – Pareto Frontier of F_{max} and l_{max} in the hot compaction process.

CONCLUSION

In this paper, we presented an optimization procedure for thermo-mechanical processes and applied it to the functional gradation of polymers. This procedure is based on advanced empirical modeling and optimization techniques. The optimization strategy was divided into two parts. At first, the procedure to generate precise and valid surrogate models was presented. The parameter preparation and suitable DOE methods were discussed. The other part focuses on the analysis and optimization of the processes. Advanced methods and tools to visualize the relevant information and to optimize the objectives were presented. These methods were exemplarily applied to two processes for functional gradation of polymers. For a uniaxial stretching process and a hot compaction process, the influence of the input parameters on the considered objectives could be quantified. It was shown that in both cases two of the four parameters had a major influence. These information were used to visualize the results and, since these parameters have a high variation, to perform a robustness analysis. Thereby a parameter setting was obtained, which enables the process be robust. Finally, the Pareto Frontier of two conflicting objectives was approximated via multi-objective optimization techniques. The estimation of the Pareto frontier can serve as a basis for selecting the processes to create the desired functionally graded properties.

ACKNOWLEDGMENTS

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REFERENCES

1. D. Biermann; K. Weinert; T. Wagner in Proc. IEEE Congr. Evolutionary Computation, 2008
2. M. D. McKay; R. J. Beckman; W. J. Conover *Technometrics*, 1979, *21*, 239
3. T. Hastie; R. Tibshirani; J. Friedman: *The Elements of Statistical Learning*, Springer, 2009.
4. B. Sieben; T. Wagner; D. Biermann in *Production Engineering. Research and Development*, 2010, *4*, 115.
5. T. Wagner; C. Bröcker; N. Saba; D. Biermann; A. Matzenmiller; K. Steinhoff in Digital Proc. Int'l Conf. Design and Analysis of Computer Experiments, St-Etienne, 2009.
6. S. Hess; T. Wagner; B. Bischl in Proceedings of the 7th International *Conference* on Learning and Intelligent OptimizatioN Conference, LION 7, 2013.
7. B. Bischl; O. Mersmann; H. Trautmann, C. Weihs in *Evolutionary Computation*, 2012, *4*, 249.
8. M. Schonlau; W. J. Welch in *Screening Methods for Experimentation in Industry, Drug Discovery and Genetics*, 2006, 308.
9. Internet resource: *Datenblatt der Fa. Bayer für Makrolon, 2805:* http://plastics.bayer.com/plastics/emea/de/produkt/makrolon/datenbaetter/Makrolon_2805_ISO/docld-78064/Makrolon_ 2805_ISO.pdf, downloaded on 20.03.2013 (2013).
10. Dr. Collin: *Technisches Datenblatt: Teach Line Reckanlage mit MDO A + Engspaltwalze + MDO B*, 2009.
11. V. Schöppner; A. Wibbeke; M. Sasse in PPS 27 Proceedings, Marrakech, 2003, CD.
12. V. Schöppner; A. Wibbeke; B. Scholtes; M. Lebsanft; W. Zinn in PPS 28 Proceedings, Pattaya, 2011, CD.
13. V. Schöppner; A. Wibbeke; M. Sasse in 70th Annual Technical Conference of the Society of Plastics Engineers (ANTEC 2012), Orlando, 2012.
14. A. K. Bledzki; H.-P. Heim; D. Paßmann; A. Ries in *Synthetic Polymer-Polymer Composites,* D. Bhattacharyya, F. Stoyko, Ed.; Carl Hanser Verlag, Munich, 2012; Vol. 1, 719-738.
15. D. Paßmann, PhD Thesis, University of Kassel, 2009.
16. H.-K. Tönshoff; B. Denkena; T. Friemuth; M. Zwick; A. Brandes in *Production Engineering. Research and Development*, 2002, *2*, 43.