View metadata, citation and similar papers at core.ac.uk
brought to you by CORE
provided by Institute of Transport Research:Publications

Efficient Determination of Material Parameters for Robust Process Simulation of Semi-crystalline Thermoplastic Composites

J. Teltschik, D. Fricke, M. Horn
Deutsches Zentrum für Luft- und Raumfahrt e.V. – German Aerospace Center, Pfaffenwaldring 38-40
70569 Stuttgart, Germany

Abstract:
Predicting material behaviour during and after consolidation using process simulation will be a decisive factor in the breakthrough of fibre reinforced high-temperature thermoplastics for primary aerospace structures. Since the materials are constantly being optimized with respect to processing and component properties, a new method is being developed to adapt existing material models for process simulations in order to quickly react to such modifications. A DoE analysis is carried out to find the model parameters with a significant effect on the process simulation which are then experimentally determined for CF/LM PAEK and implemented in an existing material model. By comparing the process-induced spring-in of vacuum-consolidated V-angles with the values derived from simulation, the adapted material model as well as the new methodology for a simplified adaptation of existing material models to novel materials is validated.

Keywords: Process Simulation, CF/LM PAEK, Thermoplastic Prepreg Tape, Process-induced Deformation, Crystallization Kinetics, Design of Experiments (DoE), Vacuum Consolidation, Aerospace

Introduction

Fibre reinforced thermoplastics (FRTP) recently gained importance for future aerospace structures. Relevant materials for primary wing or fuselage structures are carbon fibre reinforced (CF) high-performance thermoplastics such as Polyaryletherketones (PAEK) due to their promising thermomechanical properties, joining and repair potentials. However, the unique advantages of this group of materials are also countered by disadvantages such as high processing temperatures which can cause residual stresses and geometrical deviations in the final part [1].

Therefore the ability to efficiently and effectively predict material behaviour during and after consolidation will be a decisive factor in the breakthrough. A reliable process simulation will help to drastically reduce time and cost intensive iterations as well as to establish robust production processes. In this paper, in particular the process of FRTP prepreg tape consolidation under vacuum e.g. by using an oven is investigated.

Constitutive material models for FRTP that define the relations of process input parameters such as oven temperature and vacuum pressure to output parameters such as crystallinity, temperature distribution and mechanical constants, can be very complex and thus time-consuming to develop. Due to the fact that the use of FRTP for structural applications is still under development, the prepreg materials are constantly being optimized with respect to processing properties and component performance. In order to be able to react to such adaptations of the thermoplastic prepregs quickly in the view of process simulation, a new method (see Fig. 1) is developed within the scope of this work to adapt existing material models to new prepreg materials.

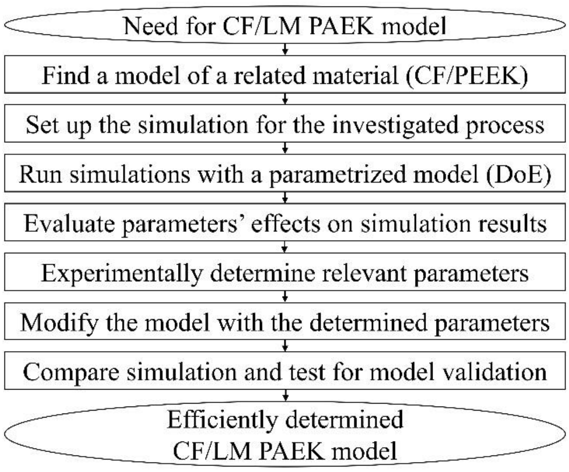

Fig. 1: *Flowchart for the performed method to efficiently obtain a new material model for FRTPs' process simulation on the basis of an existing model*

The method is being developed for the adaption of an existing approved material model of CF/PEEK to the currently investigated carbon fibre reinforced low-melt PAEK (CF/LM PAEK). For this purpose, a parameter sensitivity analysis is carried out with the aim of determining those material parameters of the existing model which have a significant effect on the results of stress-deformation analysis. Using this analysis, the number of material parameters that have to be determined for a reliable new material model can be reduced compared to designing an entirely new model. The model parameters identified as relevant are then determined for CF/LM PAEK by performing experiments on crystallization kinetics and thermomechanical properties. Subsequently, the framework of formulas and computational rules of the existing material model for CF/PEEK is supplemented by the relevant material properties of CF/LM PAEK. The resulting new material model is validated by comparing the spring-in and degree of crystallization of V-angles made of CF/LM PAEK in comparison to the values derived from process simulation.

Process Simulation

An FEM simulation for the consolidation process of CF/PEEK has been validated by Gordnian [2] and Fricke [3]. The deformations and residual stresses are thereby calculated in a stress-deformation analysis coupled to a thermo-chemical analysis which gives information about crystallization kinetics and temperature distribution during the process. The material model which is used during this simulation is a thermoelastic crystallization dependent constitutive material model for CF/PEEK and was developed by Gordnian as part of his doctoral thesis [2]. For the simulation of consolidating composite parts, the model takes into account the following phenomena as main causes for process-induced spring-in and residual stresses:

- Different coefficients of thermal expansion (CTE) of fibre and thermoplastic
- Different CTE of part and tool
- Crystallization shrinkage [2]

To define the complex interacting relations of crystallization kinetics, temperature distribution, elastic properties and thermal deformations, the model contains a framework of formulae with over 70 parameters. These parameters are characterized in differential scanning calorimetry (DSC), dynamic mechanical analysis (DMA), rheological experiments, thermogravimetric analysis (TGA) and thermomechanical analysis (TMA) on the basis of a large number of samples made of prepreg, dry fibres and neat thermoplastic [2].
To perform an adaption of the CF/PEEK model for CF/LM PAEK with minimal test effort, a sensitivity analysis on the model parameters is conducted to find the parameters with significant effect on simulation results. Therefore a simulation is set up using the Ansys 19.2 implemented software tool Compro by Convergent Manufacturing Technologies Inc. according to [4]. Here the vacuum consolidation of a rectangular V-angle with 5mm radius, 35mm width and 30mm flange length is simulated on a steel tool (see Fig. 2).

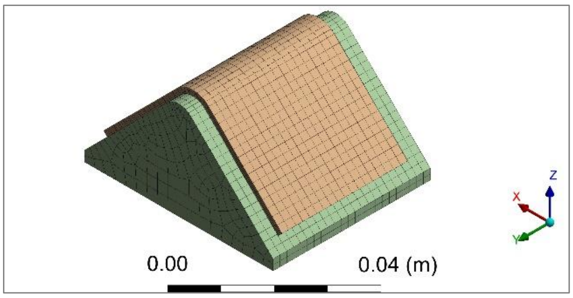

Fig. 2: *Geometry of V-angle and tool for process simulation*

A cross plied stackup [0/90/0/90//90/0/90/0] is set up in Ansys Composite PrepPost (ACP) 19.2 and the material model of CF/PEEK tape is assigned using the COMPRO implementation in Ansys Mechanical 19.2. Cooling down the Part from 390°C under vacuum it is consolidated going through melt temperature, crystallization, glass transition temperature and finally de-tooling at room temperature.
To find the model parameters with significant effect on the simulation results, the material model is parameterized and simulations with 72 variations of the model are conducted. The statistical method for defining those variations is described in the following section.

DoE for Model Parameter Analysis

For the sensitivity analysis of CF/PEEK model parameters, 33 parameters such as fibre and matrix stiffness at different temperature, coefficients of thermal expansion, matrix density at different degrees of crystallinity or crystallization kinetics parameters, are varied in accordance with a Plackett-Burman experimental design [5]. Within this experimental design, the effect of each model parameter on the simulation results degree of crystallization and spring-in of the consolidated V-angle is determined. In order to obtain a high statistical reliability, the 33 parameters are varied in 72 different experiments using the statistics software Minitab 19. For each of these simulation runs a material model with a certain variation of the model parameters has to be provided. These 72 different model variants are generated using a Python-script. After successful completion of the simulation runs, the effect of each parameter is evaluated using Pareto diagrams.

Results and Discussion

Running the process simulation of a consolidating CF/PEEK V-angle with 72 variations of material parameters, results in different final crystallinity and spring-in for each of the 72 design points. In Fig. 3 these simulated values are depicted, where a spring-in of 3° means a final angle of 87° in the composite part. The final degree of crystallinity is given as mass fraction of the thermoplastic matrix.

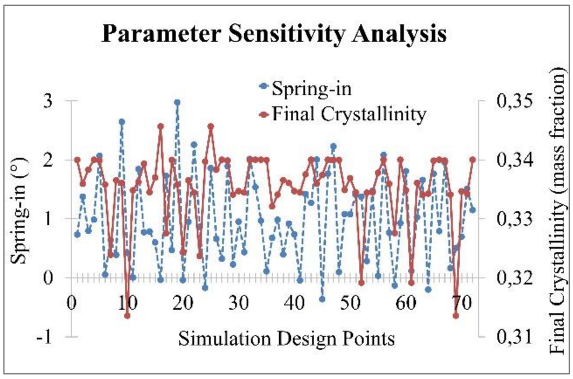

Fig. 3: *Final Crystallinity and spring-in of a consolidated V-angle for 72 design points with varied process model parameters*

Evaluating the results using the statistics software Minitab 19, the parameters with a significant effect on spring-in and crystallinity are determined in Pareto diagrams (see Fig. 4 and 5). The red dotted reference line in the Pareto diagrams is set by Minitab 19 to mark effect sizes above which a parameter is statistically significant at a significance level of 0.03.

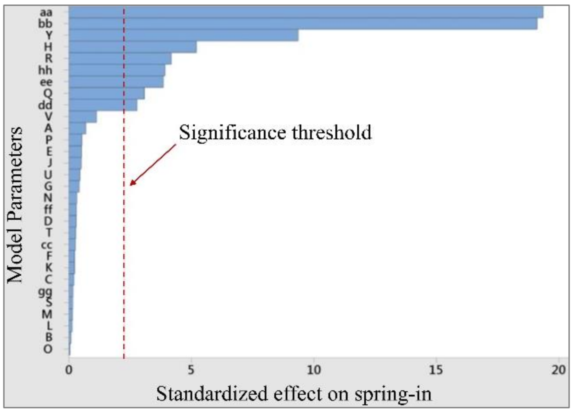

Fig. 4: *Pareto diagram showing the standardized effects of model parameters (named A to hh) on the simulated spring-in*

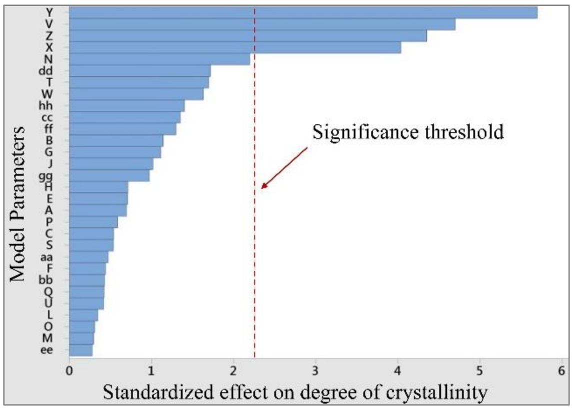

Fig. 5: *Pareto diagram showing the standardized effects of model parameters (named A to hh) on the simulated degree of crystallinity*

Evaluating the Pareto diagrams, the 33 examined model parameters, which were named from A to hh during data processing, can be narrowed down to the following eleven parameters with significant effect on the defined output variables spring-in and crystallinity:

- aa ≡ Amorphous matrix density
- bb ≡ Crystalline matrix density
- Y ≡ Matrix melting temperature
- Q ≡ Matrix glass transition temperature
- R ≡ Matrix CTE in rubbery state
- ee ≡ Matrix stiffness in glassy state
- dd ≡ Matrix Poisson's ratio in rubbery state
- V ≡ Crystallization kinetics parameter
- X ≡ Crystallization kinetics parameter
- H ≡ Longitudinal fibre stiffness
- hh ≡ Fibre volume fraction

Besides using values from material datasheets, thermal and mechanical tests are carried out to obtain these eleven characteristic parameters for CF/LM PAEK.

Emphasis must be given to the conducted DSC experiments for the crystallization kinetics analysis, as these are the key components of the thermoelastic crystallization dependent material model. Isothermal and non-isothermal crystallization experiments are conducted to investigate the dependencies of process temperature, cooling rate, degree of crystallization and crystallization rate to finally receive a model that is able to simulate the current crystallization rate at any step of the process. During the DSC experiments with different cooling rates and isothermal crystallization temperatures, the crystallization rate, current temperature and degree of crystallinity are extracted from heat flow monitoring at any point of the crystallization. Consequently, data points (blue dots/lines in Fig. 6) are obtained which represent the dependence of the crystallization rate on the current degree of crystallization and temperature. The corresponding parameters of the material model are then fitted such that the crystallization kinetics model, shown in Fig. 6 as an orange surface, is adapted to the experimental data. Data processing and model fitting is done using Wolfram Mathematica 12.

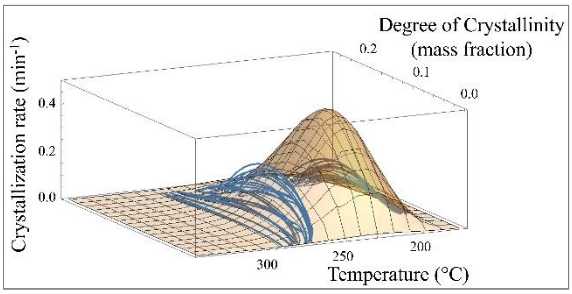

Fig. 6: *Crystallization kinetics model (orange) for LM PAEK, fitted to DSC data points (blue) representing the crystallization rate as a function of degree of crystallinity and temperature*

During process simulation the crystallization rate is stepwise integrated to calculate the current degree of crystallization, which together with the current process temperature is effecting relevant material properties such as crystallization shrinkage or matrix stiffness throughout the consolidation.

After determining all model parameters identified as relevant to the process simulation, they are integrated into the framework of the existing model to replace the previous material properties of CF/PEEK with those of CF/LM PAEK.

The resulting new material model is validated by comparing the spring-in and degree of crystallization of V-angles made of CF/LM PAEK in comparison to the values derived from process simulation. The simulation with the new material model results in a final crystallinity of 23% which agrees with the DSC experiments. The simulated spring-in is 2.1°, see Fig. 7.

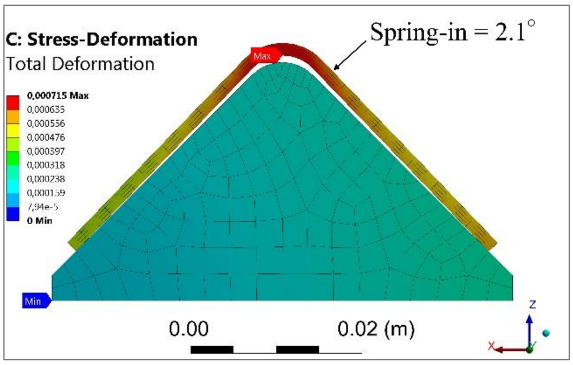

Fig. 7: *Deformed V-angle made of CF/LM PAEK after consolidation simulation using the adapted material model*

For comparison the same process simulation is performed with the initial CF/PEEK model, resulting in a crystallinity of 34% and 4.1° spring-in. The validation was done by manufacturing six V-angles by vacuum consolidation technique. Cooling the parts from 350°C to room temperature was done under vacuum pressure of approximately 0.2mbar and a cooling rate of -3K/min to -0.1K/min. The averaged spring-in of all six samples is 2.4° with a standard deviation of 0.1°, see Fig. 8.

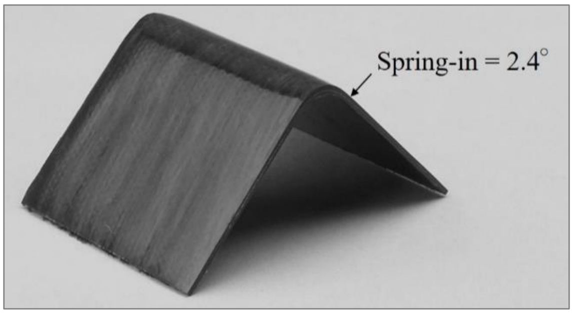

Fig. 8: *Deformed V-angle made of CF/LM PAEK in a vacuum consolidation process*

With the original model, Gordnian achieved a difference of 0.7° between simulation and real part for CF/PEEK V-angles [2]. A difference of 0.3° in spring-in between simulation and real part within this work shows that the applied method as well as the created material model for CF/LM PAEK can be recommended for further projects.

Conclusion and Outlook

The method of simplified adaptation of material models by means of parameter sensitivity analysis applied in this paper made it possible to create a valid process model for CF/LM PAEK with considerably minimized experimental effort. However, when applying this method, the user must be aware that due to performing the parameter sensitivity analysis with reference on a specific manufacturing process, the resulting material model can only be used to simulate that exact process. Here the process of vacuum consolidation was investigated. For other processes, such as automated tape laying, the material model cannot be applied without revalidation. Other material properties such as viscosity or thermal conductivity, which can theoretically be covered by the model but are not accessed in the investigated simulation investigated, could also have a significant influence on the simulation results for other processes.

In future studies, the new material model will be applied to the process simulation of larger, single and double curved parts. By comparing 3D coordinate measuring results of the process-induced deformation with the simulated deformation, the applicability of the adapted material model on full-scale structures will be validated.

Acknowledgements

The results presented here were achieved within the TRumpf research project (FKZ: 20W1721D) in the framework of the Federal Aviation Research Programme V-3, funded by the Federal Ministry for Economic Affairs and Energy, on the basis of a decision by the German Bundestag.

References

[1] T.J. Chapman, J.W. Gillespie, JR. and R.B. Pipes, Prediction of Process-Induced Residual Stresses in Thermoplastic Composites, Journal of Composite Materials, Vol. 24 (1990), 616 - 643

[2] K. Gordnian, Crystallization and Thermo-viscoelastic Modelling of Polymer Composites, University of British Columbia, Vancouver, Canada (2017)

[3] D. Fricke, G. Doll, S. Nowotny, K. Gordnian, A. Forghani, A. Poursartip, Manufacturing Simulation of the In-Situ Tape Laying Process for Thermoplastic Carbon Fiber Reinforced Tapes, SAMPE 2018

[4] Convergent Manufacturing Technologies Inc., Compro for Ansys Modelling Guidelines, Vancouver, Canada (2019)

[5] K. Siebertz, D. van Bebber, T. Hochkirchen, Statistische Versuchsplanung – Design of Experiments (DoE), VDI-Buch, Springer Heidelberg (2010)