A Consistent Environment for the Numerical Prediction of the Properties of Composite Materials

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Abstract: The current paper focuses on the creation of a consistent environment for the numerical prediction of the physical properties of polymer composite. Taking into account increasing applications of composites as well as the development of fast, reliable and cost optimized manufacturing process for those materials, the simulation becomes an important role.

A limitation factor for the successful simulation of composite processes is the correct estimation of the effective properties depending on several factors such as the constituents (fiber, polymer), the process setup.

The numerical prediction of the material properties is therefore a solution to reduce the development time by minimizing the measurement efforts.

The present prediction is based on the homogenization theory and offers more advantages compared with the analytical methods.

The tool developed here gives the possibility to fast estimate the thermal properties at different level, and to investigate their sensitivity on process induced fluctuations of the final properties.

Keywords: Composite materials, multiscale modeling, curing, homogenization, post processing

1. Introduction

Composite materials with polymer matrix play an important role in various industries such as aircraft, energy and naval industry. Considering the challenging aspects of composite manufacturing e.g. increasing of part complexity, requirements for short development time or overall cost reduction, the manufacturing process simulation (MPS) becomes an important role for the process design.

In general composite materials consist of two different materials – an embedding phase (e.g. polymer matrix) and a reinforcement phase (e.g. Filler, short or long fibre). Fibre reinforcement polymer composites (FRPC) are manufactured by different technologies that can be classified into 2 groups of dry fibre or prepreg based process family. In the case of thermosets polymer the curing step remain common for both groups. The large difference of physical properties of the involved material leads to the complexity of the process, also denoted by the modelling approaches.

The MPS can help to investigate more efficiently the need of research and optimization by providing key information at an earlier design stage. The present paper deals with an approach of a tool which function consists into the numerical prediction of physical properties as well as the optimization of process parameter based on a parametric modeling approach. In the course of high flexibility the tool offers also the possibility to solve multiscale applications by defining and using a representative volume element (RVE). All this aspects are merged in one tool called CHAMAELEON.

CHAMAELEON combines the features of MATLAB® and COMSOL Multiphysics®. The GUI (Graphic User Interface) of MATLAB® enables the customized settings of the problem to be solved or of the property to be computed respectively. The parametric geometry definition offers the possibility to investigate the sensitivity of a given property such as the dependency of the thermal conductivity from the fibre content. The input data from the GUI are then used to solve a field problem within the COMSOL environment. The calculation made in COMSOL is used in the sense of a numerical homogenization. The final properties of the defined RVE are obtained by a numerical integration of the subdomain value of each constituent and volume average.

2. Description of the Tool

CHAMAELEON presents different settings options such as settings for geometric parameters or for physical properties. At the geometric panel the user can choose one of the multiscale modeling level. In each level the data of the respective geometry can be easily changed and adapted on the problem. This offers an individual handling and a high flexibility of the tool.
The access of the physical properties occurs over different scripts written in COMSOL Multiphysics which can be called from the GUI environment. In the current case the focus was set on the thermal properties. An extension for other physical areas such as mechanical or electric properties is also possible.

CHAEMELEON is mainly developed for the composite sector, where the quality of the part is depending on the fiber volume content.
The fibre volume content is adjustable and depends on the packing density of the fibers. In general the maximum fiber content value accounts from 0.79 using a quadratic packing to 0.91 using a hexagonal packing as depicted in Figure 1.

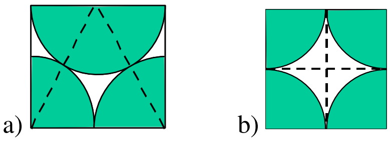

Figure 1. a) hexagonal packing
b) quadradic packing

However in reality, there will be a combination of both packing densities.

The parameterization of the input values allows the customer to adjust the fiber volume content. Therewith the costumer gains the information about the influence of the fiber volume content on the curing process of the sample.

2.1 Multiscale modeling

For improving the properties of FRCP material, the view from the global composite structure (macro plane) to the RVE (micro plane) gives a better understanding of the material behavior inside the part, which helps to get information about the complete laminate structure [1].

a) Macroscale

The simulation in the macrolevel acts as a possibility for a fast analysis of the thermal transfer of the entire system depending on the sizing and design of the tool. Different tool design such as one-sided tool concepts in additional with auxiliary supplies sketched in Figure 2 or completely closed tools, have different influence on the thermal gradients of the entire structure.

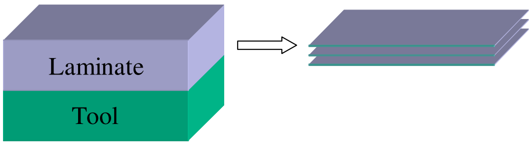

Figure 2. Macrolevel: Laminated structure

The properties of the laminate are proportionately composed of the properties of the respective components.
Equ.1 – Equ.4 shows the composite properties – density ρ_l, thermal conductivity in and cross the fiber direction λ_l, λ_t and the heat capacity c_p – by the rule of mixture [2,3]:

$$\rho_l = v_f * \rho_f + (1 - v_f) * \rho_m \qquad \text{Equ.1}$$

$$\lambda_l = v_f * \lambda_f + (1 - v_f) * \lambda_m \qquad \text{Equ.2}$$

$$\lambda_t = \frac{\lambda_{fl} \lambda_m}{v_f \lambda_m + v_m \lambda_{ft}} \qquad \text{Equ.3}$$

$$c_{p_l} = \frac{v_f * \rho_f * c_{pf} + (1 - v_f) * \rho_m * c_{pm}}{v_f * \rho_f + (1 - v_f) * \rho_m} \qquad \text{Equ.4}$$

where v_f stands for the fibre volume content, ρ_f , ρ_m represent the respective density as well as λ_f, λ_m and c_{pf}, c_{pm} the thermal conductivity respectively the heat capacity values of the constituent parts. The index l and t stand for longitudinal respectively transversal.

Using the macrolevel can also show that the process-setup involves different materials. Following the macroscale level serves for a fast estimation of the manufacturing concept.

b) Meso/Microscale

In contrast the meso/microlevel focuses on the material behavior of the components inside. It comes to a differentiation of the laminate from the macroscale into a RVE for a combination of fibre and matrix. Here the properties of the components can be individually allocated as depicted in Figure 3.

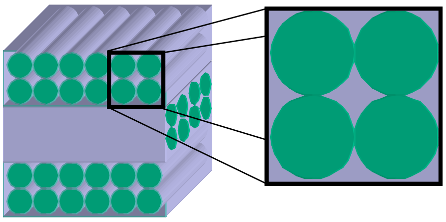

Figure 3. Meso/microlevel: fibre and matrix

Using the meso/microlevel allows the analysis of several materials with their different properties. In the present case the thermal behavior and the curing kinetics were the main aspect of this research. As soon as the behavior of the material inside is known it can be transformed to the complete system.

2.2 Parameterization

The feature of the parameterization of the model at each level allows the customized adaptation on the current problem. This is an enrichment compared to the exclusive application of COMSOL multiphysics. With the combination of the features of COMSOL Multiphysics and the use of the GUI from MATLAB there is originated an efficient tool for the analysis regarding the behavior particular of composite material.

For example in the microlevel the geometry of the model is adaptable depending on the fiber content as can be seen in Figure 4 and Figure 5.

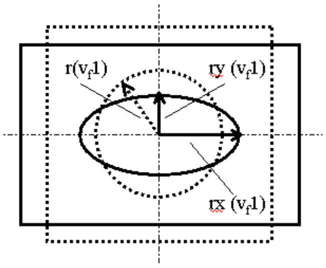

Figure 4. Parameterization of the fibre geometry

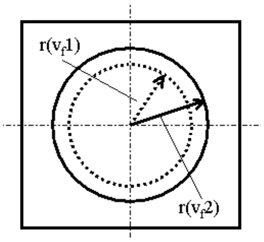

Figure 5. Parameterization of the fibre radius depending on the fibre content

Also the grade of impregnation of the fibre tows can be regarded by changing the size of merging zone displayed in Figure 6.

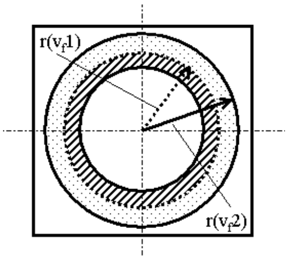

Figure 6. Parameterization of merging zone

3. Use of COMSOL Multiphysics

COMSOL Multiphysics offers in general a good environment for the analysis of material behavior. Therefore it serves as basic for the tool.

3.1 Equation

The principle of the numerical homogenization is demonstrated by solving the heat transfer problem. At the microscale, the problem consists into predicting first the temperature distribution within a RVE and in a second step to calculate the resulting thermal conductivity. For this purpose the heat transfer module of COMSOL Multiphysics is used (Equ.5).

Heat Transfer by Conduction

$$\rho C_p \frac{dT}{dt} - \nabla \cdot (k \nabla T) = Q \qquad \text{Equ.5}$$

At the macroscale, the computing domain consists into a section through the system mould and laminate (assembly of single plies). The thermal properties computed at the microlevel are used as input for the laminate. The exothermic curing reaction of the resin is modeled by an ordinary different equation 1st order from Kamal Sourour type (Equ.6) [4,5]:

$$\frac{d\alpha}{dt} = (k \cdot \alpha^m)(1-\alpha)^n \qquad \text{Equ.6}$$

where α is the degree of curing and m, n are the reaction orders. k denotes the temperature dependency of the reaction and are given by an Arrhenius approach (Equ.7):

$$k = A \cdot \exp(\frac{-E}{RT}) \qquad \text{Equ.7}$$

Equ.6 has been implemented into COMSOL by using the PDE general mode (Equ.8):

$$e\frac{\partial^2 u}{\partial t^2} + d\frac{\partial u}{\partial t} + \nabla \cdot \Gamma = F \qquad \text{Equ.8}$$

and by identifying the coefficients as follows:

$$e = 0, \quad d = 1, \quad \Gamma = 0,$$
$$F = (k \cdot \alpha^m)(1-\alpha)^n$$

As output from the calculation, the temperature at various locations over the entire process time are obtained and automatically plotted.

4. Result and discussion

The post processing capability of COMSOL enables a customized interpretation and representation of the results. Figure 7a and 7b demonstrate typical results computed by CHAMEALEON. Concerning the microscale case Figure 7a shows the comparison of the numerical and analytical results of the effect of the fibre content ϕ on the thermal conductivity of the composite $\lambda_{comp.}$ As can be seen a good agreement between analytical and numerical prediction has been obtained.

Figure 7b represents the macroscale solution. It illustrates the temperature evolution of the tool as well as of the composite material with different fibre content values during the curing process. The interpretation of the predicted temperature evolution enables the optimization of the process set-up.

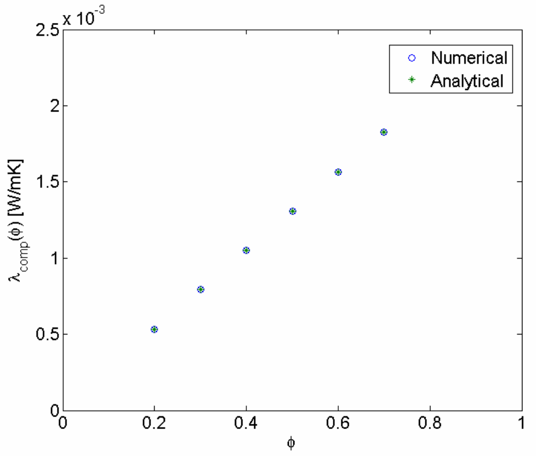

Figure 7a. Microscale (*Thermal Conductivity as function of fibre content*).

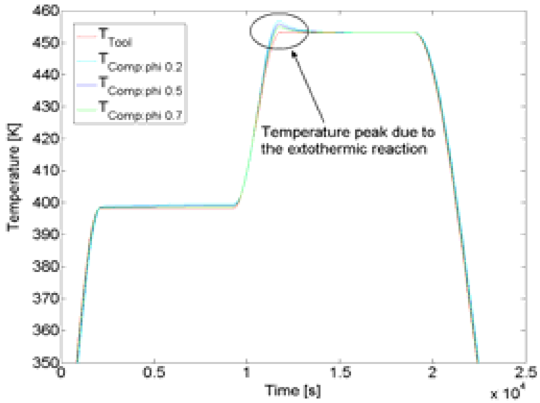

Figure 7b. Macroscale (*Influence of the exothermic reaction on the temperature evolution*).

5. Conclusions

The program CHAMAELEON has been designed especially for users interested on fast investigation of the influence on global laminate properties as well as on the optimization of the process parameter (heating and cooling rates). The principle of CHAMAELEON depicted in this work by the thermal properties can be easily extended to other physical properties like moisture behavior, mechanical or electrical properties. Compared with the classical way of process modeling, the use of CHAMAELEON can help to reduce the modeling effort on a significant manner.

6. Future prospects

The further developing of CHAMAELEON will concern with the illustration of the 3D model of each level. In addition the implementation of more complex geometries created for example in the textile geometric modeller TexGen developed at the University of Notthingham should be realizable [6]. However, this approach would possibly postulate a developing of COMSOL regarding the compatibility of COMSOL and TexGen.

7. References

1. Kwan, J.W., Allen D.H., Talreja R., M*ultiscale modeling simulation composite materials and structures*, Springer, New York (2008)
2. Aström, B.T., *Manufacturing of Polymer Composites*, p.150. Chapman and Hall, London (1997)
3. Krishan, K. Chawla, *Composite Materials Science and Engineering*, p.324. Springer, New York (1998)
4. Osswald, Tim, *Polymer Processing-Modeling and Simulation*, p.62f., Hanser, München (2006)
5. Michaud, J. Dennis, *Simulation-based design optimization and control of thick composite laminates manufactured by resin transfer molding*, p.62f., University of Delaware, Delaware (2000)
6. Schubel, P.J., Warrior, N.A., Rudd, C.D., Surface Roughness Modeling of Textile Composites Using TexGen*, 8th International Conference on Textile Composites,* Nottingham, UK, (16-18 Oct 2006)