

Fiber-Orientation-Evolution Models for Compression Molding of Fiber Reinforced Polymers

Róbert Bertóti^{1*} and Thomas Böhlke¹

Micro Abstract

This presentation gives a short review on the Fiber-Orientation-Evolution models commonly used in commercial softwares. The basis of the considered models is Jeffery's equation from 1922 which describes the motion of a single ellipsoidal particle in a Newtonian fluid. The later models extend Jeffery's equation for many fiber system, with the use of Fiber-Orientation-Tensors. Models are discussed up to the o-iARD-RPR model (Tseng 2016), and compared considering representative flow modes.

¹Chair for Continuum Mechanics, Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

*Corresponding author: robert.bertoti@kit.edu

Introduction

The anisotropic mechanical properties of a discontinuous fiber reinforced polymer part mainly depend on the fiber orientation distribution. To forecast the direction dependent properties, the production process has to be simulated which is commonly injection- or compression molding. The next session gives an overview of the several, so-called fiber orientation evolution models which were developed in the last few decades. Two of these models are implemented and compared considering representative flow modes and different closure approximations. Through the Abaqus VUMAT (Vectorized User Material) interface the Folgar-Tucker model with the quadratic closure is implemented and applied for the compression molding of a plate.

Model equations

Jeffery's equation

The foundation for all considered fiber orientation evolution models is Jeffery's equation [6] which describes the motion of a single ellipsoidal particle in a Newtonian fluid

$$\dot{\mathbf{n}}_\alpha = \bar{\mathbf{W}}[\mathbf{n}_\alpha] + \bar{\xi}(\bar{\mathbf{D}}[\mathbf{n}_\alpha] - (\mathbf{n}_\alpha \otimes \mathbf{n}_\alpha \otimes \mathbf{n}_\alpha)[\bar{\mathbf{D}}]) \quad , \quad \bar{\xi} = \frac{\bar{a}^2 - 1}{\bar{a}^2 + 1} \quad , \quad \bar{a} = \bar{l}/\bar{d}. \quad (1)$$

The normalized orientation vector of a fiber α is noted with \mathbf{n}_α and $\dot{\mathbf{n}}_\alpha$ indicates the material derivative of it. The effective vorticity and rate-of-deformation tensors are $\bar{\mathbf{W}}$ and $\bar{\mathbf{D}}$, respectively. The geometry factor $\bar{\xi}$ is defined through the aspect ratio \bar{a} of a representative fiber with the length \bar{l} and diameter \bar{d} . The dyadic product is noted with \otimes and a linear mapping with $[\]$. A modern derivation of Jeffery's equation can be found in [7].

Numerically it is more efficient to use fiber orientation tensors [1] instead of modeling each of the fibers. The empirical, reducible second and fourth order fiber orientation tensors of the first kind [8], belonging to M pieces of fibers, are defined as

$$\bar{\mathbf{N}} = \frac{1}{M} \sum_{\alpha=1}^M \mathbf{n}_\alpha \otimes \mathbf{n}_\alpha \quad , \quad \bar{\mathbf{N}} = \frac{1}{M} \sum_{\alpha=1}^M \mathbf{n}_\alpha \otimes \mathbf{n}_\alpha \otimes \mathbf{n}_\alpha \otimes \mathbf{n}_\alpha. \quad (2)$$

With the use of these fiber orientation tensors Jeffery's equation can also be written in a tensorial form

$$\dot{\bar{\mathbf{N}}}^h = \bar{\mathbf{W}}\bar{\mathbf{N}} - \bar{\mathbf{N}}\bar{\mathbf{W}} + \bar{\xi}(\bar{\mathbf{D}}\bar{\mathbf{N}} + \bar{\mathbf{N}}\bar{\mathbf{D}} - 2\bar{\mathbf{N}}^*[\bar{\mathbf{D}}]). \quad (3)$$

The upper index h indicates that (3) describes the reorientation for the case that only hydrodynamic forces are acting. The fourth order fiber orientation tensor $\bar{\mathbf{N}}$ is marked with a * in (3), because different approximations can be used to calculate it. The simplest one is the quadratic closure [4]

$$\bar{\mathbf{N}}^{\text{Quad}} = \bar{\mathbf{N}} \otimes \bar{\mathbf{N}}. \quad (4)$$

This formula is only exact for unidirectional fiber orientation distributions. For more precise calculations, in this paper, the Invariant Based Optimal Fitting (IBOF) closure [3]

$$\bar{\mathbf{N}}^{\text{IBOF}} = \bar{\beta}_1 \text{sym}(\mathbf{1} \otimes \mathbf{1}) + \bar{\beta}_2 \text{sym}(\mathbf{1} \otimes \bar{\mathbf{N}}) + \bar{\beta}_3 \text{sym}(\bar{\mathbf{N}} \otimes \bar{\mathbf{N}}) + \bar{\beta}_4 \text{sym}(\mathbf{1} \otimes \bar{\mathbf{N}}\bar{\mathbf{N}}) + \bar{\beta}_5 \text{sym}(\bar{\mathbf{N}} \otimes \bar{\mathbf{N}}\bar{\mathbf{N}}) + \bar{\beta}_6 \text{sym}(\bar{\mathbf{N}}\bar{\mathbf{N}} \otimes \bar{\mathbf{N}}\bar{\mathbf{N}}) \quad (5)$$

is used. The rule, how to calculate $\bar{\beta}_i$, $i = 1 \dots 6$, as a function of the second and third invariants of $\bar{\mathbf{N}}$, is given in [3]. The $\text{sym}(\cdot)$ operator calculates the symmetric part of its argument and $\mathbf{1}$ notes the second order identity tensor. There are several other types of closure approximations which are not considered in this paper.

Extensions of Jeffery's equations

To consider the effect of the fiber-fiber interaction Folgar and Tucker (FT) [5] added an isotropic rotary diffusion term to (3)

$$\dot{\bar{\mathbf{N}}}^{\text{FT}} = \dot{\bar{\mathbf{N}}}^h + 2\bar{C}_1\dot{\bar{\gamma}}(\mathbf{I} - 3\bar{\mathbf{N}}) \quad , \quad \dot{\bar{\gamma}} = \sqrt{2(\bar{\mathbf{D}} \cdot \bar{\mathbf{D}})} \quad , \quad \bar{C}_1 = \bar{f}(\bar{c}_f). \quad (6)$$

The FT model predicts too fast fiber reorientation in comparison to experiments. To slow down the fiber reorientation Wang et al. introduced the Reduced Strain Closure (RSC) model [11]. To be able to predict Anisotropic Rotary Diffusion (ARD) Phelps and Tucker introduced the ARD model [9] which can be combined with the RSC model. The ARD-RSC model includes 6 phenomenological parameters. To reduce the number of these parameters Tseng et al. introduced the objective improved ARD model with Retarding Principal Rate (o-iARD-RPR) [10] which contains only 4 phenomenological parameters.

Numerical implementation and results

Representative flow modes

The tensorial form of Jeffery's equation (3) and the Folgar-Tucker model (6) are implemented with the quadratic (4) and IBOF closures and compared for representative flow cases. The investigated shear, elongational, compressional and planar flow cases are the same as described in [2]. The initial fiber orientation distribution is isotropic. The similarities and differences of the four investigated models are represented here on the example of the \bar{N}_{xx} component vs. the von Mises equivalent strain ε_M , considering the shear (Figure 1a)) and the elongational (Figure 1b)) flow.

2D Eulerian press model

A fluid material model is implemented through the VUMAT interface. This fluid model is tested for simple shear, elongation and compression, with the help of a one element Lagrangian model, and it is proven that the numerical results match the analytical solutions.

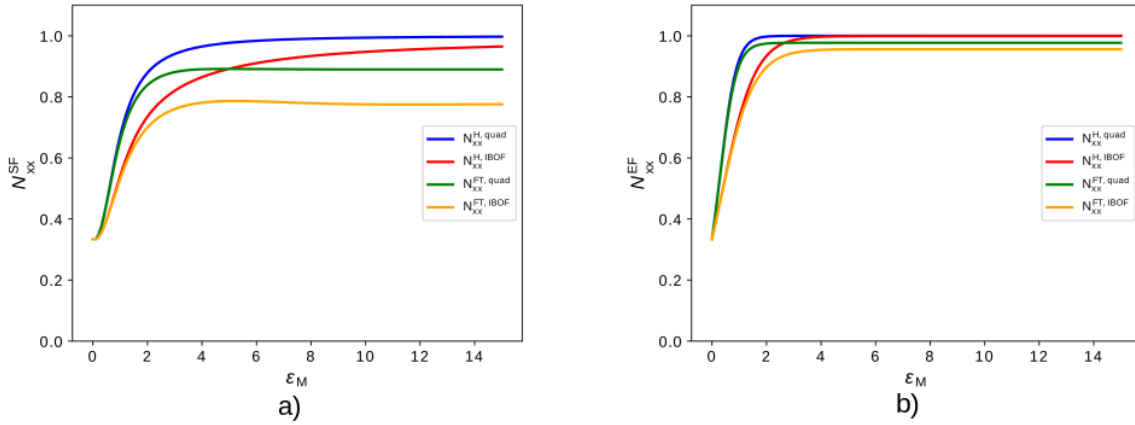


Figure 1. The evolution of the the \bar{N}_{xx} component in a) shear flow and b) in elongational flow

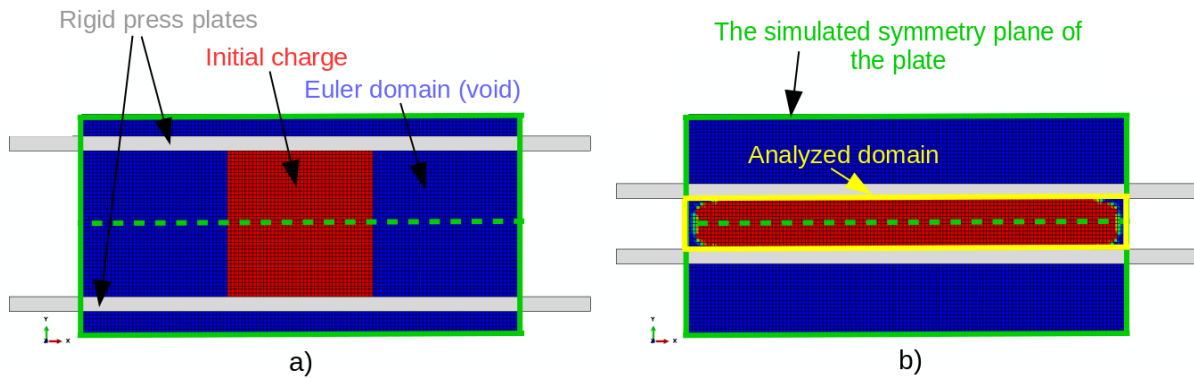


Figure 2. 2D Eulerian press model in Abaqus, a) initial state, before compression, b) end state, after compression

For the 2D Eulerian press model the Folgar-Tucker equation (6) with the quadratic closure (4) are implemented. The 2D, Eulerian press model is depicted in Figure 2.

The initial fiber orientation distribution is planar isotropic in the x - y plane. The final spatial distribution of the diagonal components of \bar{N} are represented in Figure 3.

Conclusions

With the introduced 2D Eulerian press model the shell-core-shell fiber orientation layers can be analyzed, and all of the constitutive equations can be modified. The shell layer is not modeled correctly yet, because the actual model does not consider the high temperature gradients at the contact surface of the press plate and the compressed material. The model can be developed to investigate the effect of the anisotropic effective viscosity [2].

Acknowledgements

This work was partially supported by the German Research Foundation (DFG) within the International Research Training Group “Integrated engineering of continuous-discontinuous long fiber reinforced polymer structures” (GRK 2078).

References

- [1] S. G. Advani and C. L. Tucker III. The use of tensors to describe and predict fiber orientation in short fiber composites. *Journal of Rheology*, 31(8):751–784, 1987.

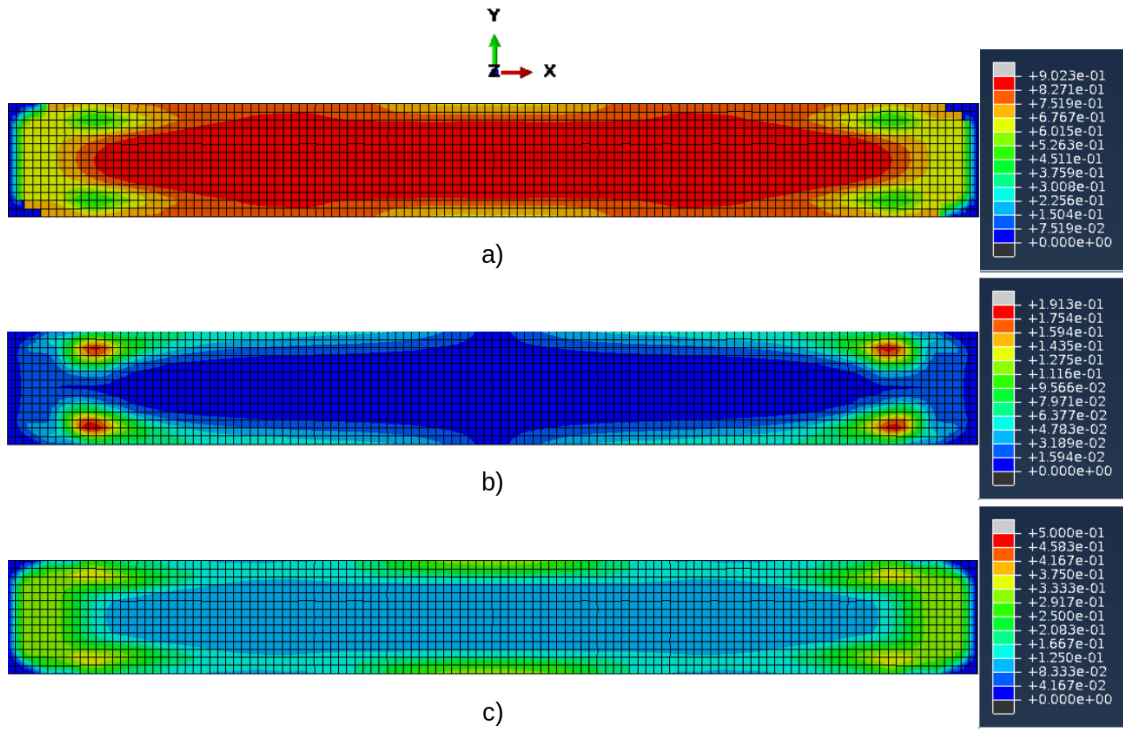


Figure 3. Spatial distribution of the diagonal components of $\bar{\mathbf{N}}$ in the analyzed domain, a) \bar{N}_{xx} component, b) \bar{N}_{yy} component, c) \bar{N}_{zz} component

- [2] R. Bertóti and T. Böhlke. Flow-induced anisotropic viscosity in short frps. *Mechanics of Advanced Materials and Modern Processes*, 3(1):1–12, 2017.
- [3] D. H. Chung and T. H. Kwon. Invariant-based optimal fitting closure approximation for the numerical prediction of flow-induced fiber orientation. *Journal of rheology*, 46(1):169–194, 2002.
- [4] M. Doi. Molecular dynamics and rheological properties of concentrated solutions of rodlike polymers in isotropic and liquid crystalline phases. *Journal of Polymer Science: Polymer Physics Edition*, 19:243, 1981.
- [5] F. Folgar and C. L. Tucker III. Orientation behavior of fibers in concentrated suspensions. *Journal of reinforced plastics and composites*, 3(2):98–119, 1984.
- [6] G. B. Jeffery. The motion of ellipsoidal particles immersed in a viscous fluid. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, volume 102, pages 161–179. The Royal Society, 1922.
- [7] M. Junk and R. Illner. A new derivation of Jeffery’s equation. *Journal of Mathematical Fluid Mechanics*, 9(4):455–488, 01 2007.
- [8] K.-I. Kanatani. Distribution of directional data and fabric tensors. *International Journal of Engineering Science*, 22(2):149–164, 1984.
- [9] J. H. Phelps and C. L. Tucker. An anisotropic rotary diffusion model for fiber orientation in short-and long-fiber thermoplastics. *Journal of Non-Newtonian Fluid Mechanics*, 156(3):165–176, 2009.
- [10] H.-C. Tseng, R.-Y. Chang, and C.-H. Hsu. An objective tensor to predict anisotropic fiber orientation in concentrated suspensions. *Journal of Rheology*, 60(2):215–224, 2016.
- [11] J. Wang, J. F. O Gara, and C. L. Tucker III. An objective model for slow orientation kinetics in concentrated fiber suspensions: Theory and rheological evidence. *Journal of Rheology*, 52(5):1179–1200, 2008.