

**TITLE:** Virtual parametrisation of fibre orientation models based on microscopic flow simulations

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**ABSTRACT:**

Today's material systems of discontinuous fibre reinforced polymers often contain a high fibre content, due to mechanical performance. Therefore, their rheological behaviour and producibility is complex and dominated by fibre-fibre interactions, which also crucially affect the resulting fibre orientation. Hence, complex fibre orientation models are needed to describe the re-orientation of fibres during mould filling, which often depend on (semi-)empirical model parameters. These parameters must be approximated with surrogate models or based on experiments, which includes high effort and only applies for specific cases. Such models, used in a process simulation for a whole part, are normally formulated for second-order orientation tensors, as presented by Advani and Tucker [1]. Therefore, a representative orientation distribution is modelled instead of the orientation of every single fibre. The two orientation evolution models regarded in this work are the Folgar-Tucker-Equation (FTE) presented by Folgar and Tucker [2] and developed to describe the fibre orientation in concentrated suspensions, and the so called ARD-RSC model [3], developed by Phelps and Tucker for highly filled long fibre systems.

This work presents a method to determine the needed model parameters by comparing the tensorial model solution to micro-scale simulation results, containing flexible and interacting individual fibres. The micro-scale simulations are performed with the smoothed particle hydrodynamics (SPH) method as shown in Figure 1. To do so, the approach of Meyer et al. [4] is adapted and applied for longer fibres and larger model domains. For macro-model parameter determination, pure shear is simulated on both scales. Multiple SPH results are averaged, and the resulting orientation tensor is calculated. Afterwards, the FTE and ARD-RSC are fitted to these results over time, as exemplary given in Figure 2.

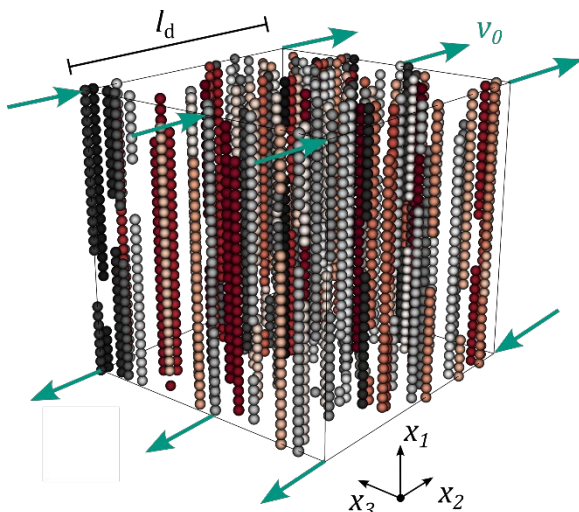


Figure 1: Example of micro-model SPH simulation with individual fibres that are initially aligned unidirectionally. Matrix phase is present but not visible. [5]

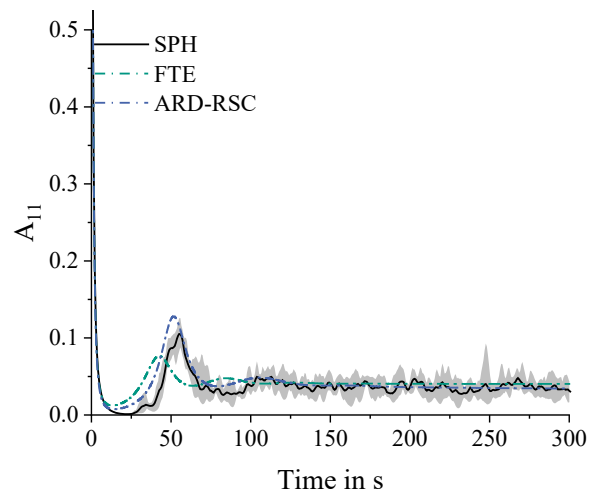


Figure 2: Comparison of calculated fibre orientation tensor value  $A_{11}$  of SPH simulation (black), fitted Folgar-Tucker approach (green) and fitted ARD-RSC approach (blue). [5]

Based on this parametrisation, the macro-scale process simulations of a 2 mm thick rectangular plate with a central sprue are regarded. FTE and ARD-RSC models and compared to injection moulding experiments, represented by CT-scans to determine the fibre orientation. The experiments are performed with a 10 vol.-% short glass fibre reinforced phenolic compound. The macro-scale simulations are performed non-isothermal,

with an anisotropic non-Newtonian viscosity model [6]. The results of the parameterised models are compared to the CT-scans and to identical models, where the parameters are determined according to the state of the art (SoA) as shown in Figure 3.

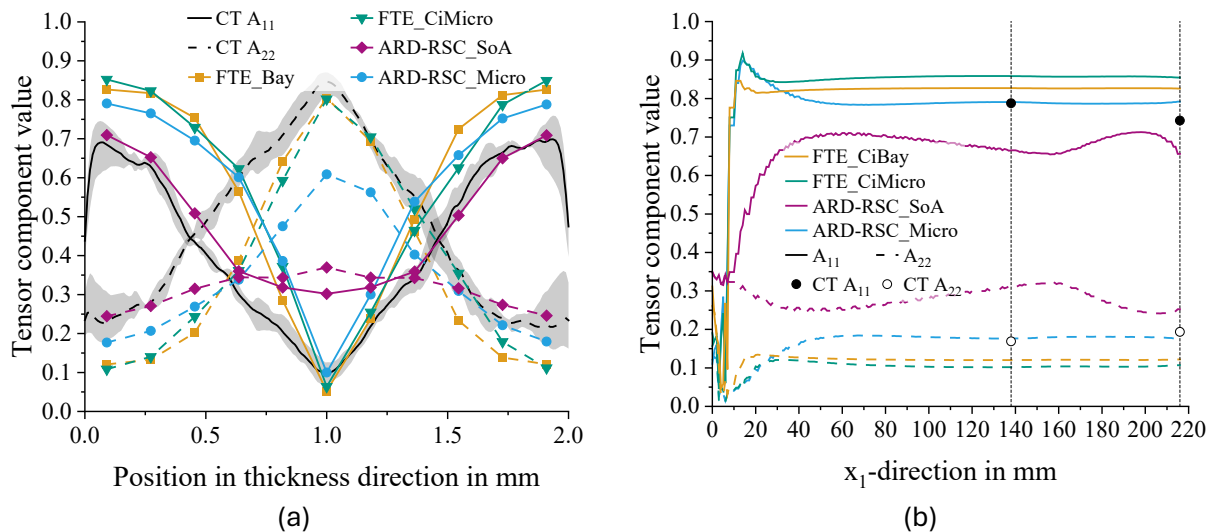


Figure 3: Comparison of fibre orientation tensor components  $A_{11}$  (solid lines) and  $A_{22}$  (dashed lines) from macroscale simulations and CT-Scans. Results over the plate's thickness (a) and along the flow path (b). CT-results in black (including min/max in grey), Folgar-Tucker approach with  $C_{1,Bay}$  (orange) and fitted  $C_1$  (green), the ARD-RSC approach with state-of-the-art parameters (purple) and fitted ARD-RSC approach (blue). [5]

The predicted orientation distribution is more similar to the experimental results, if the fitted parameters are used, showing identical tendencies over the complete plate's thickness, although the state-of-the-art ARD-RSC is closer to the experimental data in some points. Furthermore, the runs with fitted parameters show a more dynamic behaviour, containing local maxima and minima along the flow path, which is also visible in the micro simulations, but not for SoA parameters of the ARD-RSC model. Therefore, the presented approach enables the parameterisation of complex orientation models, based on virtual data and hence also over a longer period of time, without the need of experimental data.

## References

- [1] Advani SG, Tucker CL. The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites. *Journal of Rheology* 1987;31:751–84. <https://doi.org/10.1122/1.549945>.
- [2] Folgar F., Tucker C.L. Orientation Behavior of Fibers in Concentrated Suspensions. *Journal of Reinforced Plastics and Composites*, Vol 3 1984:98–119.
- [3] Phelps JH, Tucker CL. An anisotropic rotary diffusion model for fiber orientation in short- and long-fiber thermoplastics. *Journal of Non-Newtonian Fluid Mechanics* 2009;156:165–76. <https://doi.org/10.1016/j.jnnfm.2008.08.002>.
- [4] Meyer N, Saburow O, Hohberg M, Hrymak AN, Henning F, Kärger L. Parameter Identification of Fiber Orientation Models Based on Direct Fiber Simulation with Smoothed Particle Hydrodynamics. *J Compos Sci* 2020;4:77. <https://doi.org/10.3390/jcs4020077>.
- [5] Wittemann F, Hof L, Kärger L. Using microscale SPH-simulations to parameterize macroscopic fiber orientation models for discontinuous fiber reinforced polymers. *Multiscale and Multidiscip Model Exp and Des* 2025;8:445. <https://doi.org/10.1007/s41939-025-01043-3>.
- [6] Wittemann F, Maertens R, Kärger L, Henning F. Injection molding simulation of short fiber reinforced thermosets with anisotropic and non-Newtonian flow behavior. *Composites Part A: Applied Science and Manufacturing* 2019;124:105476. <https://doi.org/10.1016/j.compositesa.2019.105476>.