

Virtual parametrisation of fibre orientation models based on microscopic flow simulations

Lightweight Engineering



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1. Fundamentals

- Motivation
- Fibre orientation modelling
- Parametrisation methods

2. SPH micro-scale simulations

- Model built-up
- Sensitive analysis
- Results for parametrisation

3. Macro-scale results

- Parameter fitting
- Validation

4. Summary

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Fundamentals

Motivation

- Fibres in suspensions move during mould filling
- Fibres and matrix interact and influence each other
- Fibres re-orientate depending on material and process



“Processing controls [macroscopic] properties by affecting fibre orientation, so we want to predict fibre orientation.”

Charles L. Tucker III (source: University of Illinois)

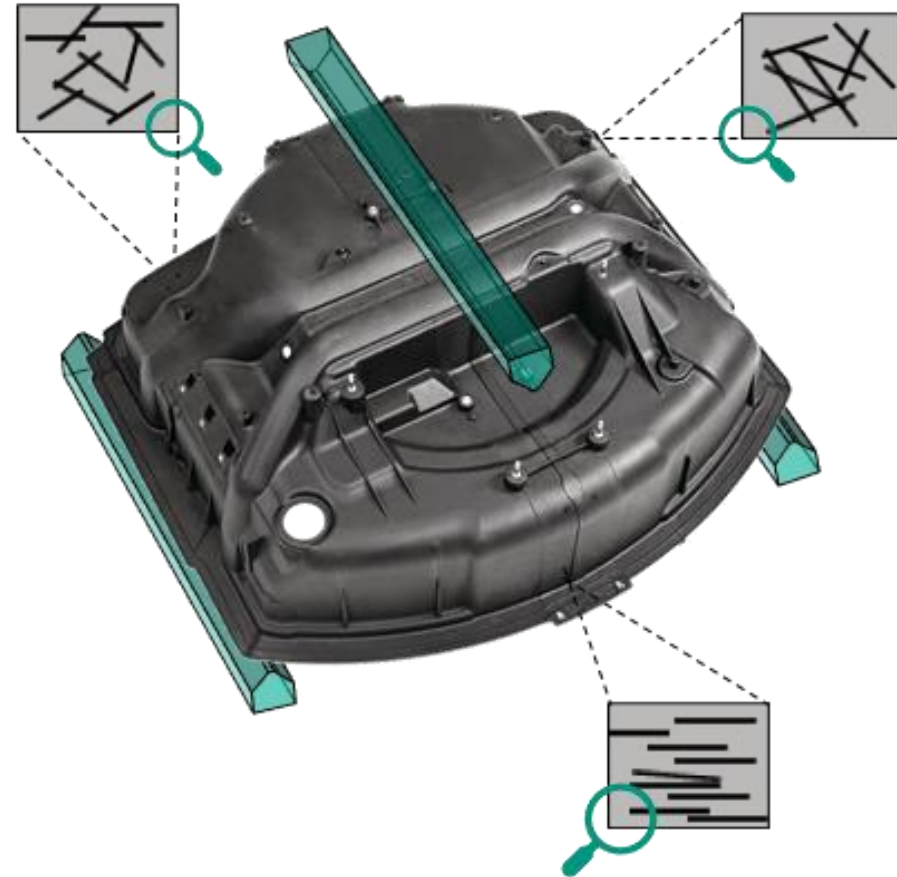
source: Lanxess AG

Fundamentals

Motivation

- Today's orientation models need empirical parameters
- Existing approaches to predict these parameters often only consider the stationary orientation state
(Advani 1994, Tucker 2022)
- Injection moulded parts often consist of direction changes and short flow paths
- Stationary orientation state is not reached in most regions of the part
- Time dependent data is hard to get experimentally

The aim is to find and verify parameters for orientation models over time



source: Lanxess AG

Fundamentals

Fibre orientation modelling

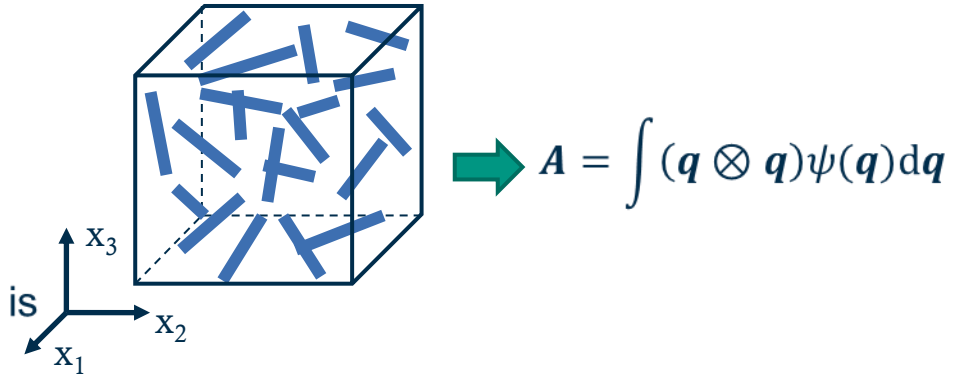
- Most of today's approaches for fibre orientation modelling use second order orientation tensors \mathbf{A} according to Advani and Tucker (Advani and Tucker 1987)

- Only a representation of the "average" orientation in the considered volume is calculated

- Most of today's models are based on the work of Jeffery for the rotation of a single ellipsoid (Jeffery 1922)

- Jeffery Equation for orientation tensors:

$$\frac{d\mathbf{A}}{dt} + \mathbf{U} \frac{\partial \mathbf{A}}{\partial \mathbf{x}} = -(\mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W}) + \frac{r_f^2 - 1}{r_f^2 + 1} \{\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D} - 2\mathbb{A}\mathbf{D}\}$$



\mathbf{q} : Single fiber vector
 \mathbf{A} : Second order fiber orientation tensor
 \mathbb{A} : Fourth order fiber orientation tensor
 ψ : probability density function
 \mathbf{U} : Velocity vector
 \mathbf{W} : Vorticity tensor
 \mathbf{D} : Strain-rate tensor
 r_f : Fiber aspect ratio

Fundamentals

Fibre orientation modelling

- Jeffery Equation was developed for single inclusion and only works well for dilute suspensions
- Extensions for higher fibre volume fractions and longer fibres were developed
- The two approaches considered in this work are:
 - Folgar-Tucker-approach: *(Folgar and Tucker 1984)*

$$\frac{d\mathbf{A}}{dt} + \mathbf{U} \frac{\partial \mathbf{A}}{\partial \mathbf{x}} = -(\mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W}) + \frac{r_f^2 - 1}{r_f^2 + 1} \{\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D} - 2\mathbf{A}\mathbf{D}\} + 2C_1\dot{\gamma}(\boldsymbol{\delta} - 3\mathbf{A})$$

- ARD-RSC-approach: *(Wang et al. 2008, Phelps and Tucker 2009)*

$$\frac{d\mathbf{A}}{dt} + \mathbf{U} \frac{\partial \mathbf{A}}{\partial \mathbf{x}} = -(\mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W}) + \frac{r_f^2 - 1}{r_f^2 + 1} \{\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D} - 2[\mathbb{A} + (1 - \kappa)(\mathbb{L} - \mathbb{M}\mathbf{A})]\mathbf{D}\} + \dot{\gamma}[2[\mathbf{C} - (1 - \kappa)\mathbb{M}\mathbf{C}] - 2\kappa(\mathbf{C} \cdot \boldsymbol{\delta})\mathbf{A} - 5(\mathbf{C}\mathbf{A} + \mathbf{A}\mathbf{C}) + 10[\mathbb{A} + (1 - \kappa)(\mathbb{L} - \mathbb{M}\mathbf{A})]\mathbf{C}]$$

$$\text{with: } C_{ij} = b_1\boldsymbol{\delta} + b_2\mathbf{A} + b_3\mathbf{A}\mathbf{A} + \frac{b_4}{\dot{\gamma}}\mathbf{D} + \frac{b_5}{\dot{\gamma}^2}\mathbf{D}\mathbf{D}$$

$\dot{\gamma}$: Scalar shear rate
 $\boldsymbol{\delta}$: Second order Unity tensor
 \mathbb{L}, \mathbb{M} : Fourth order tensors depending on \mathbf{A}
 κ : Strain reduction factor (empirical)
 C_1 : Interaction coefficient (empirical)
 \mathbf{C} : Interaction tensor (empirical)
 b_{1-5} : Empirical parameters

Fundamentals

Parametrisation methods

- There are different approaches to determine C_I for the Folgar-Tucker-approach, for example:

- Phan-Tien (*Phan-Tien et al. 2002*)

$$C_{I,PT} = 0.03(1 - \exp(-0.224\phi_f r_f))$$

- Bay (*Bay 1991*)

$$C_{I,Bay} = 0.0184 \exp(-0.7148\phi_f r_f)$$

- According to Heinen 2007, it is common to use $C_{I,PT}$ for $\phi_f r_f \leq 1.3$ and $C_{I,Bay}$ for $\phi_f r_f > 1.3$ (*Heinen 2007*)
- For more complex approaches like the ARD-RSC, fitting to experiment or using literature data is used to determine the parameters (*Tucker 2022*)

Aim of this work: Find an experimental-free method to determine parameters for the ARD-RSC approach

ϕ_f : Fibre volume fraction
 r_f : Fibre aspect ratio

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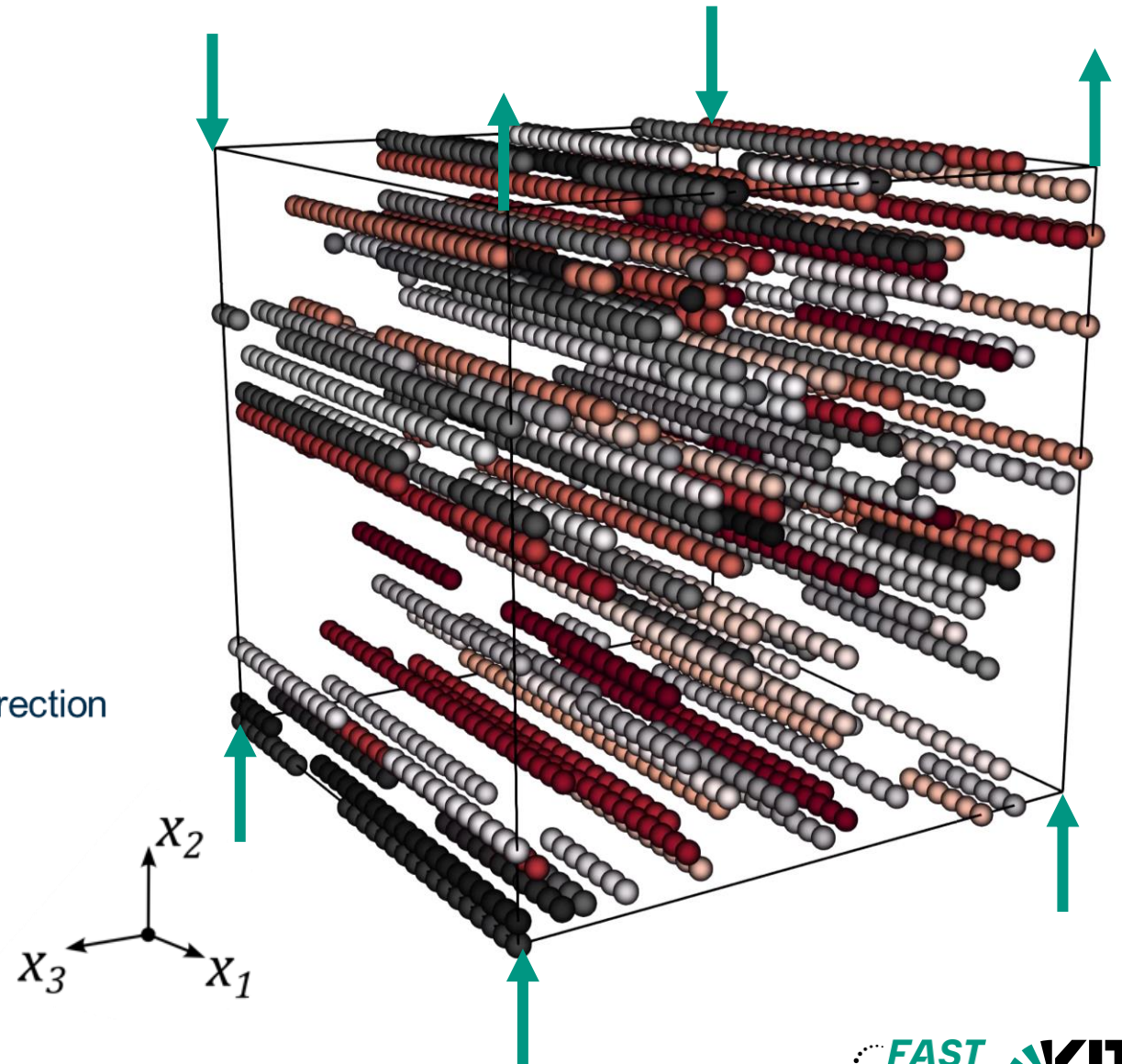
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SPH micro-scale simulations

Model built-up

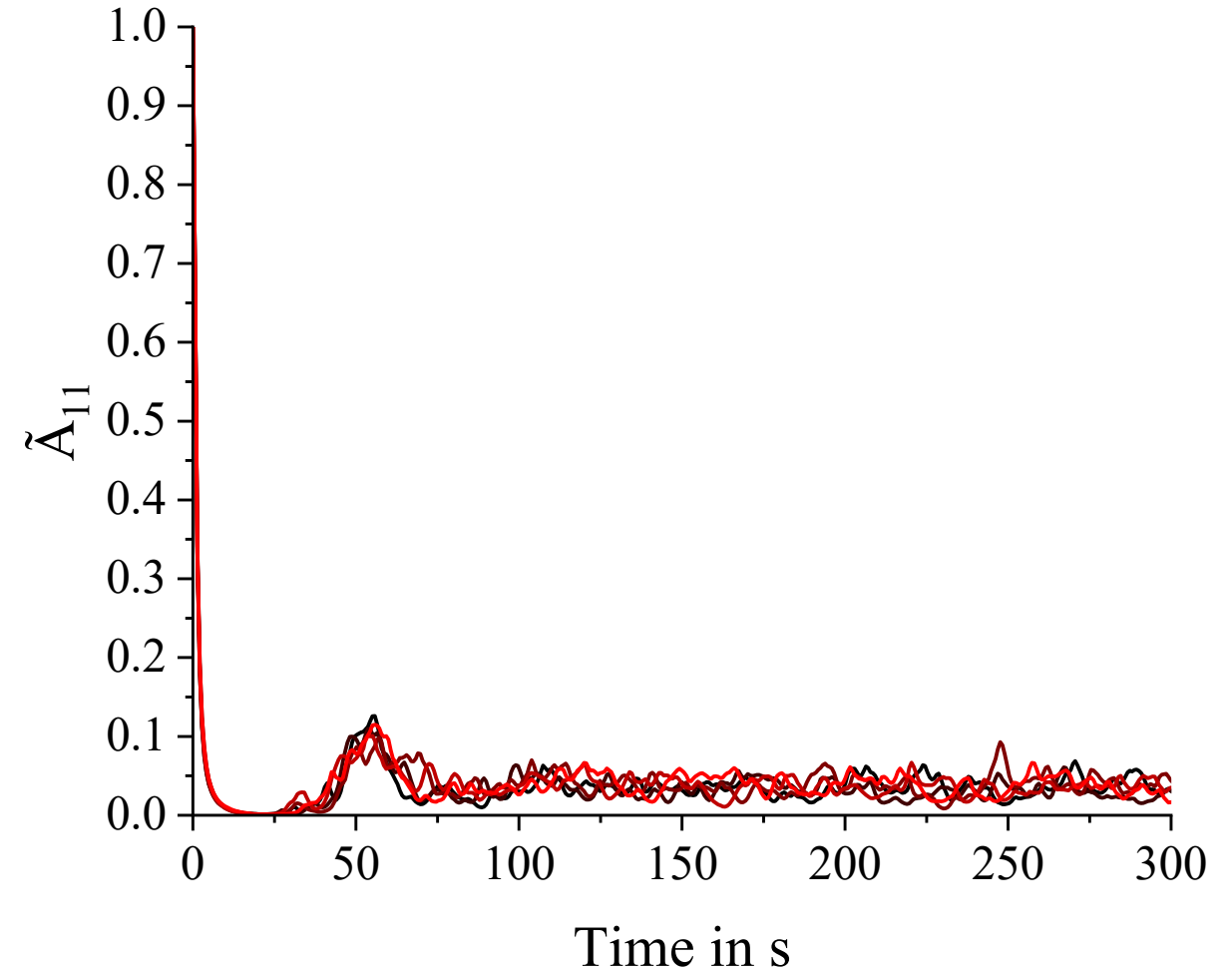
- SPH micro-model with individual and bendable fibres in Newtonian fluid under shear (*Witte mann et al. 2025*)
 - Fibre volume fraction $\phi_f=0.1$
 - Fibre aspect ratio $r_f=22.1$
- Method based on work of Meyer et al. (*Meyer et al. 2020*)
- Fibre particles are connected to approximate stiffness
Fluid particles are viscous
- Initial fibre placement is random, but all fibres point in x_1 -direction
- Quick orientation in x_2 -direction
- Fibres start bending and interacting



SPH micro-scale simulations

Sensitive analysis – Initial fibre placement

- Identical simulations to evaluate the influence of random fibre placement
- Re-orientation peak around 50 s appears quite similar in time and amplitude
 - Fibres do not directly go into steady-state
- Influence of initial state detectable but not significant

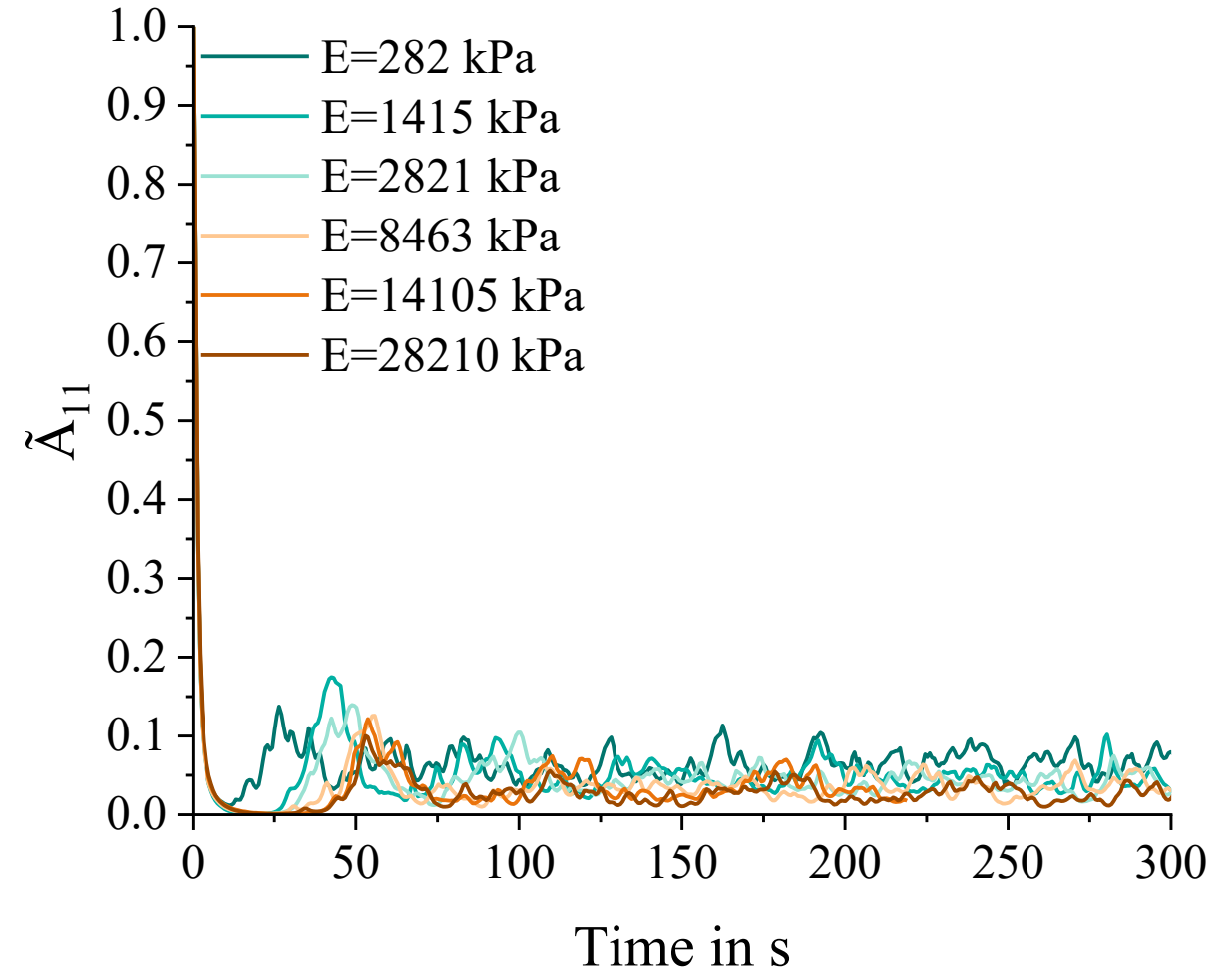


(Wittemann et al. 2025)

SPH micro-scale simulations

Sensitive analysis – fibre stiffness

- Identical simulations for different fibre stiffness
 - Real stiffness can not be achieved
- Lower stiffness leads to an earlier reorientation peak (green lines)
- No change detectable for higher stiffnesses (yellow to red)
- Stiffness of 8463 kPa represents good option for numerical efficiency and fibre representation

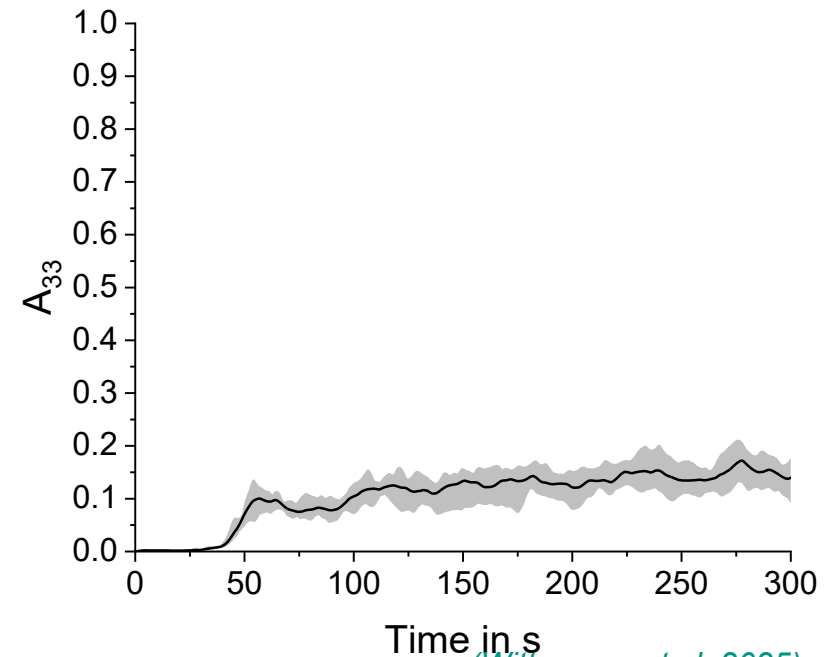
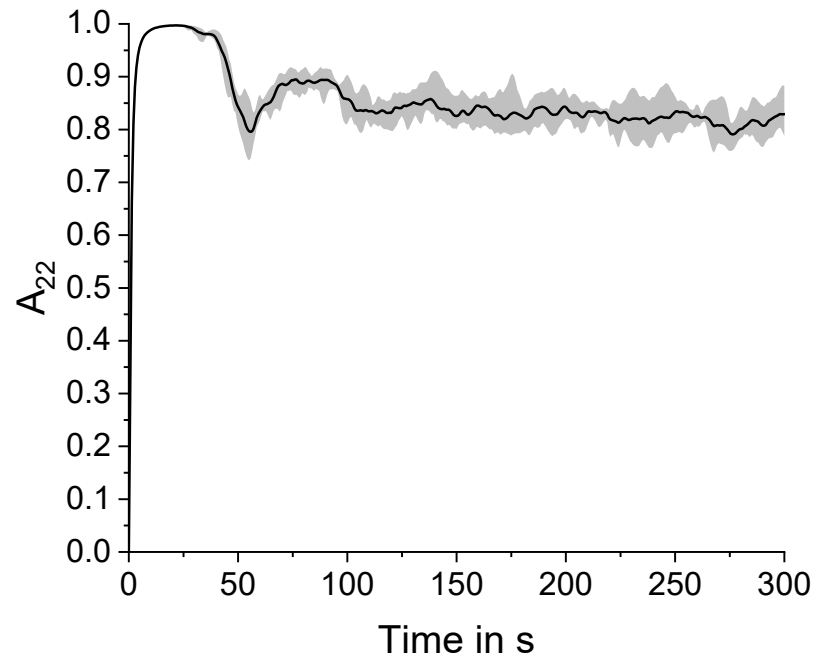
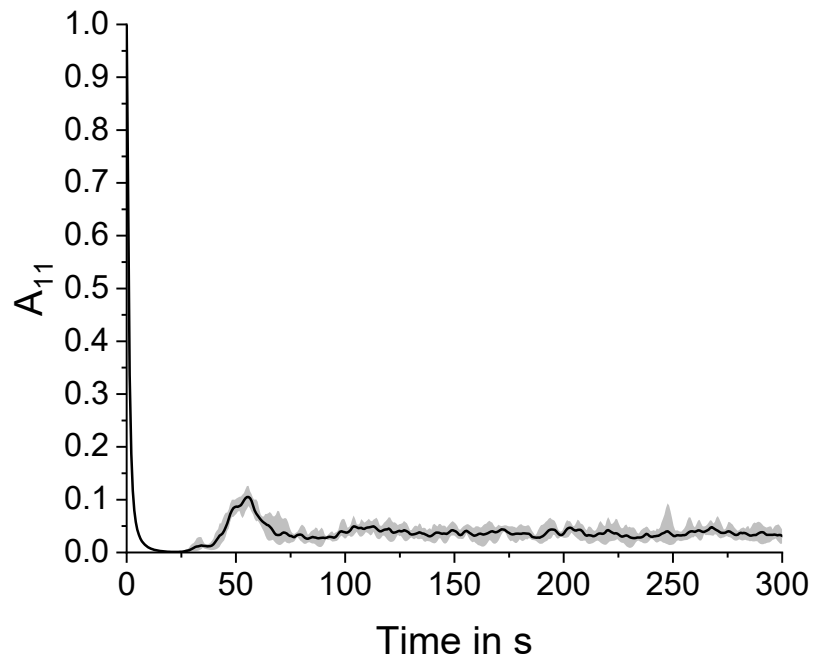


(Wittemann et al. 2025)

SPH micro-scale simulations

Results for parametrisation

- Average of 5 simulations with stiffness of 8463 kPa, resulting tensor of the whole domain is used as objective function
- Reorientation peak of A_{11} about 50 s, rise of A_{33} after about 30 s



(Wittemann et al. 2025)

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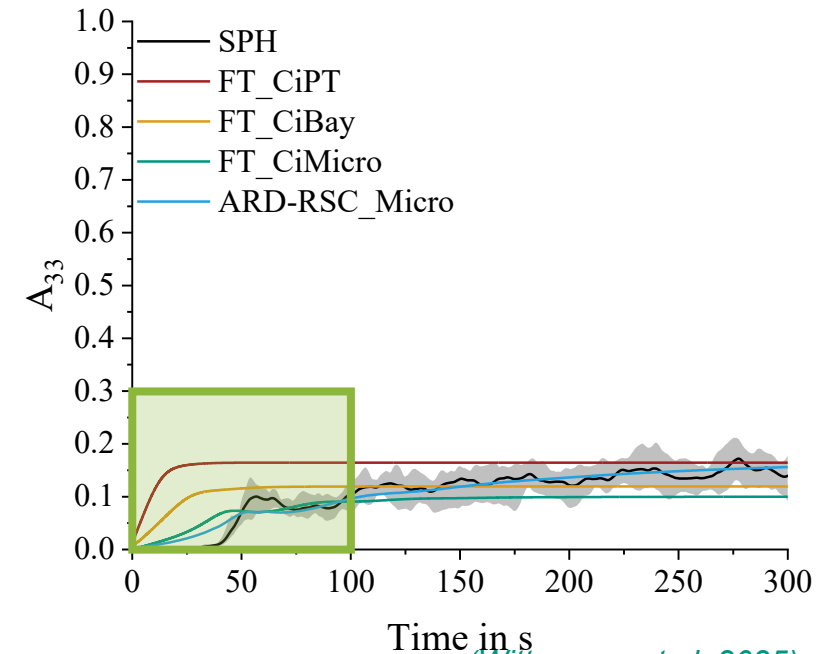
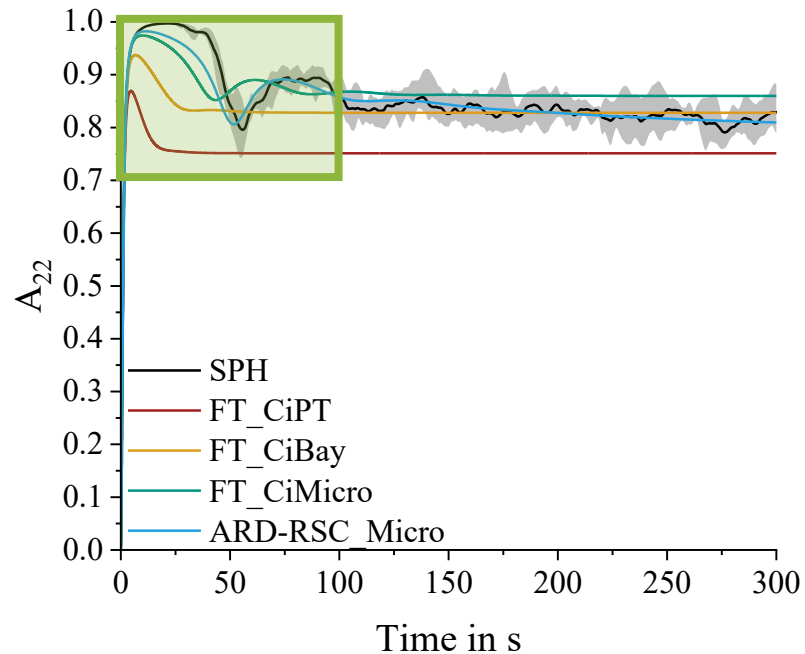
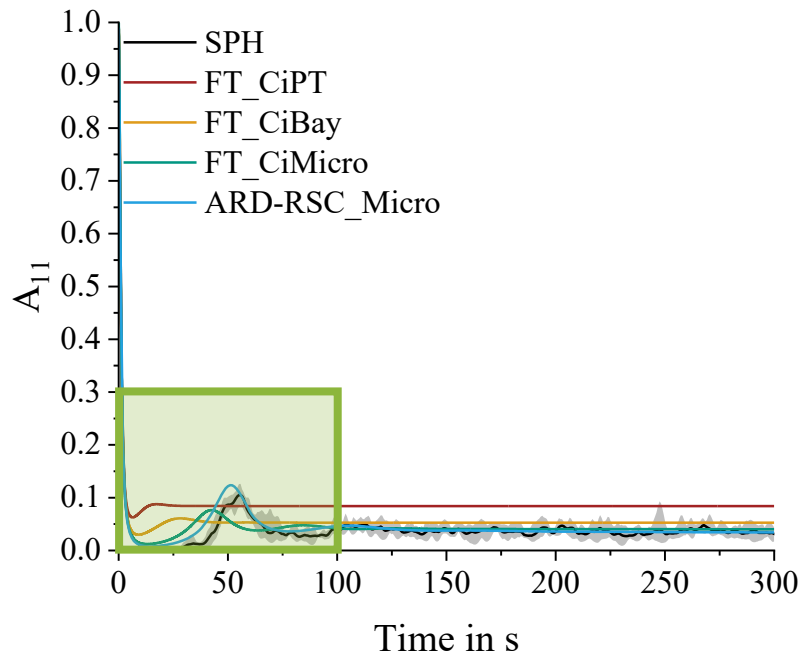
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Macro-scale results

Parameter fitting

- Besides ARD-RSC all approaches predict stationary state too early
- Bay predicts stationary state quite well
- Only ARD-RSC approach predicts reorientation peak and rise of A_{33} correct in time and amplitude

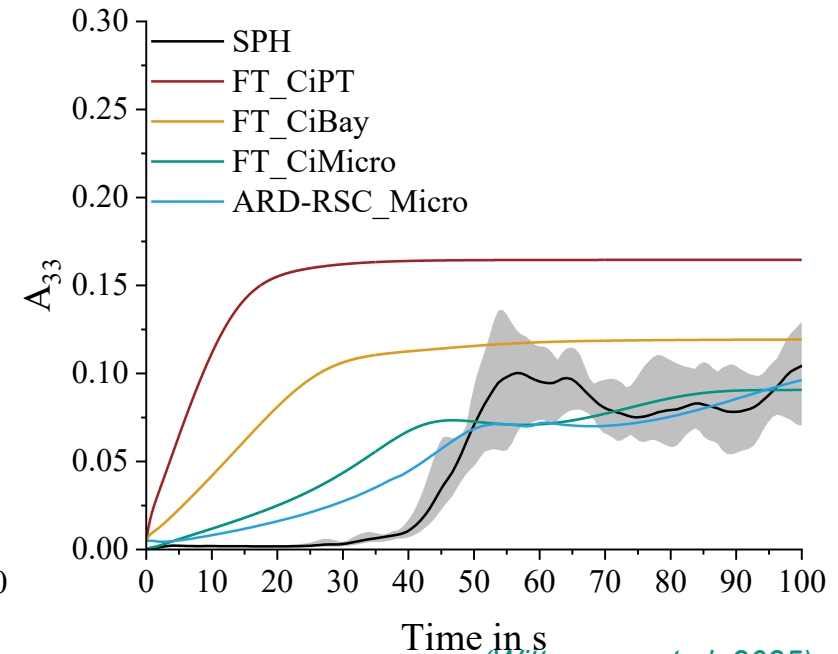
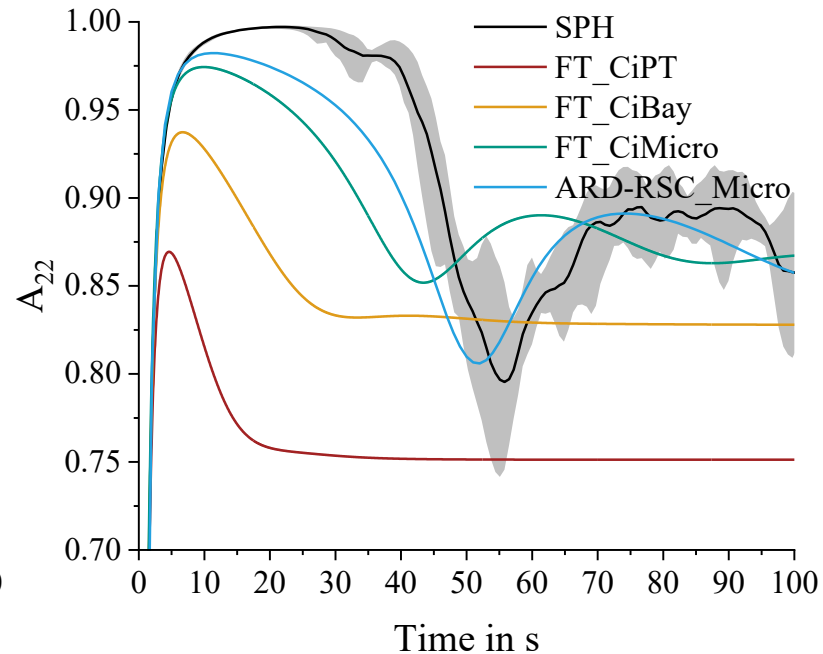
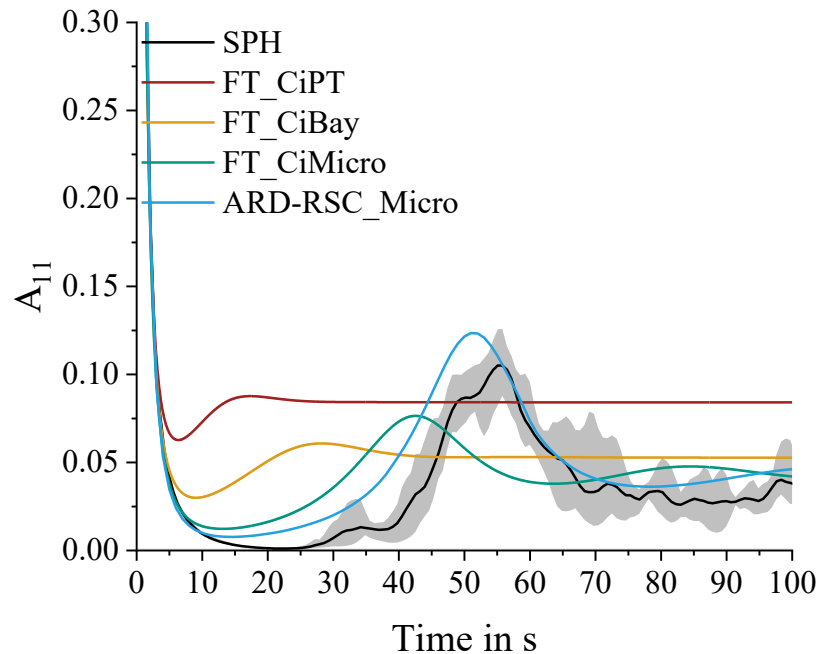


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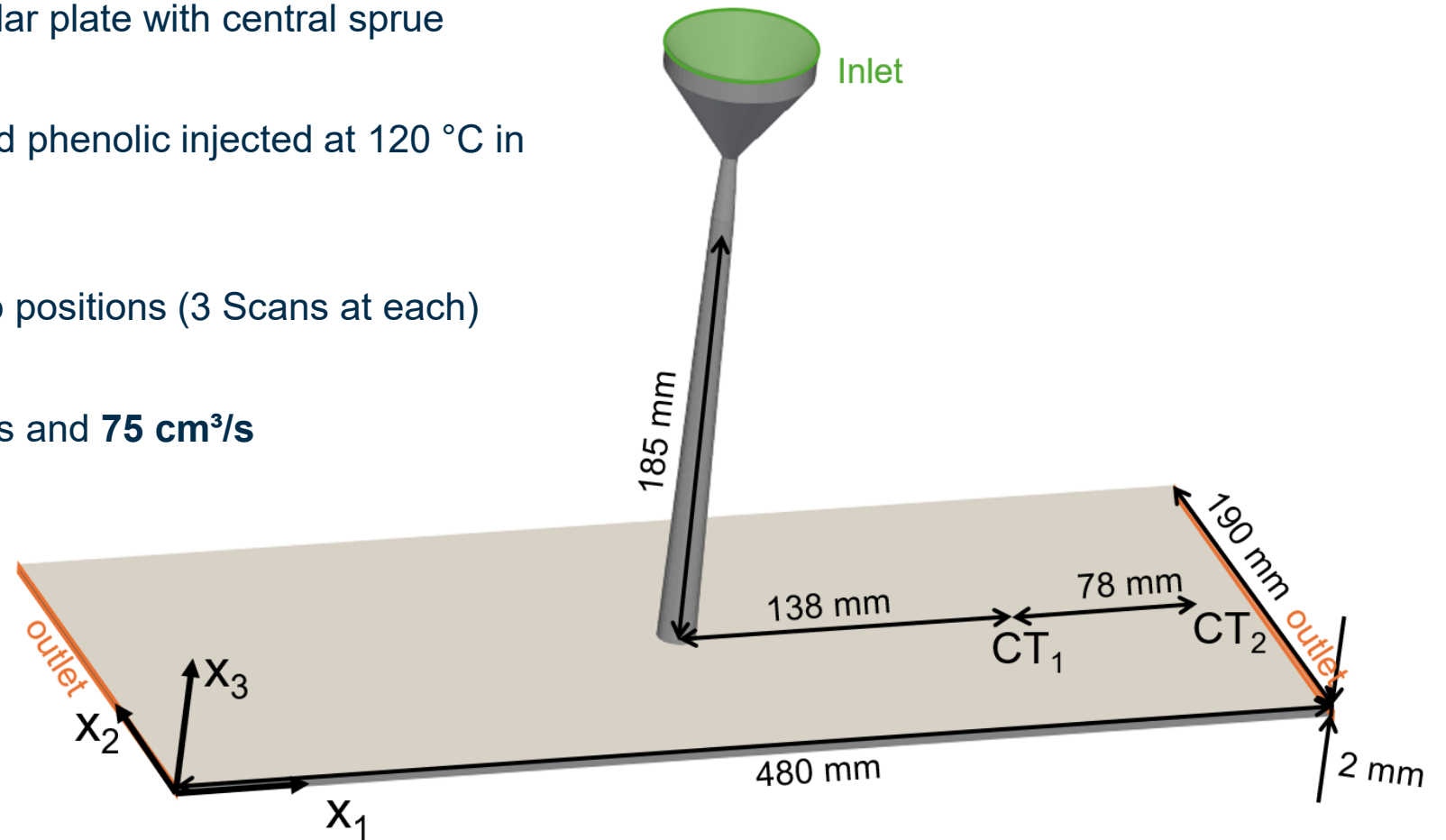


(Wittemann et al. 2025)

Macro-scale results

Validation

- Injection moulding trials of rectangular plate with central sprue
- 10 vol.-% short glass fibre reinforced phenolic injected at 120 °C in 175 °C tool
- Fibre orientation via CT-Scan at two positions (3 Scans at each)
- Two different filling speeds: 50 cm³/s and **75 cm³/s**

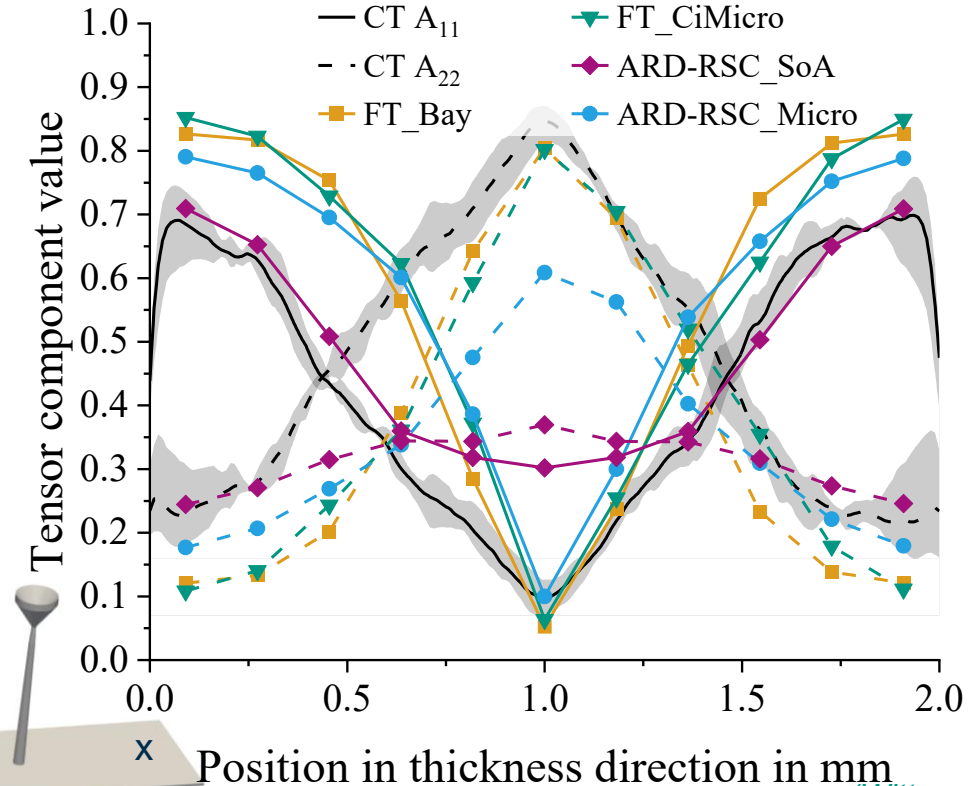
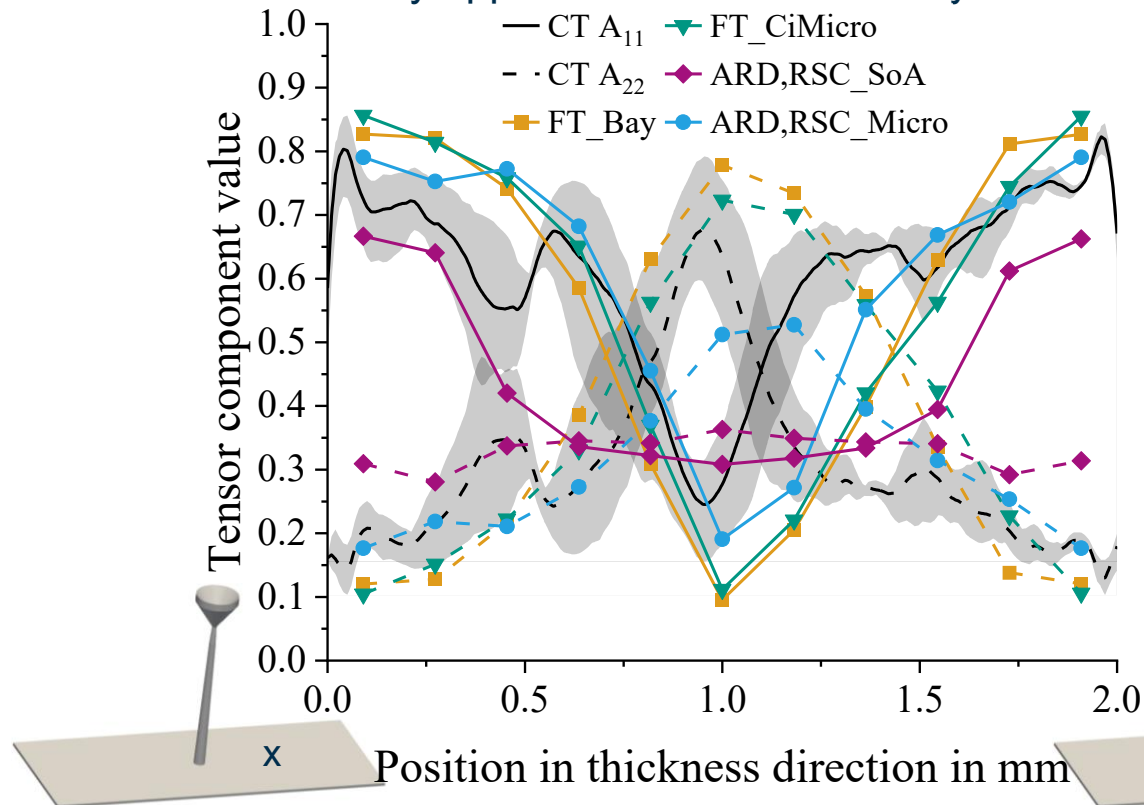


(Witte mann et al. 2025)

Macro-scale results

Parameter fitting

- Results for 75 cm³/s over plate thickness
- Non-monotonous and asymmetric progression of experimental results at CT₁
- Fitted ARD-RSC only approach with this tendency

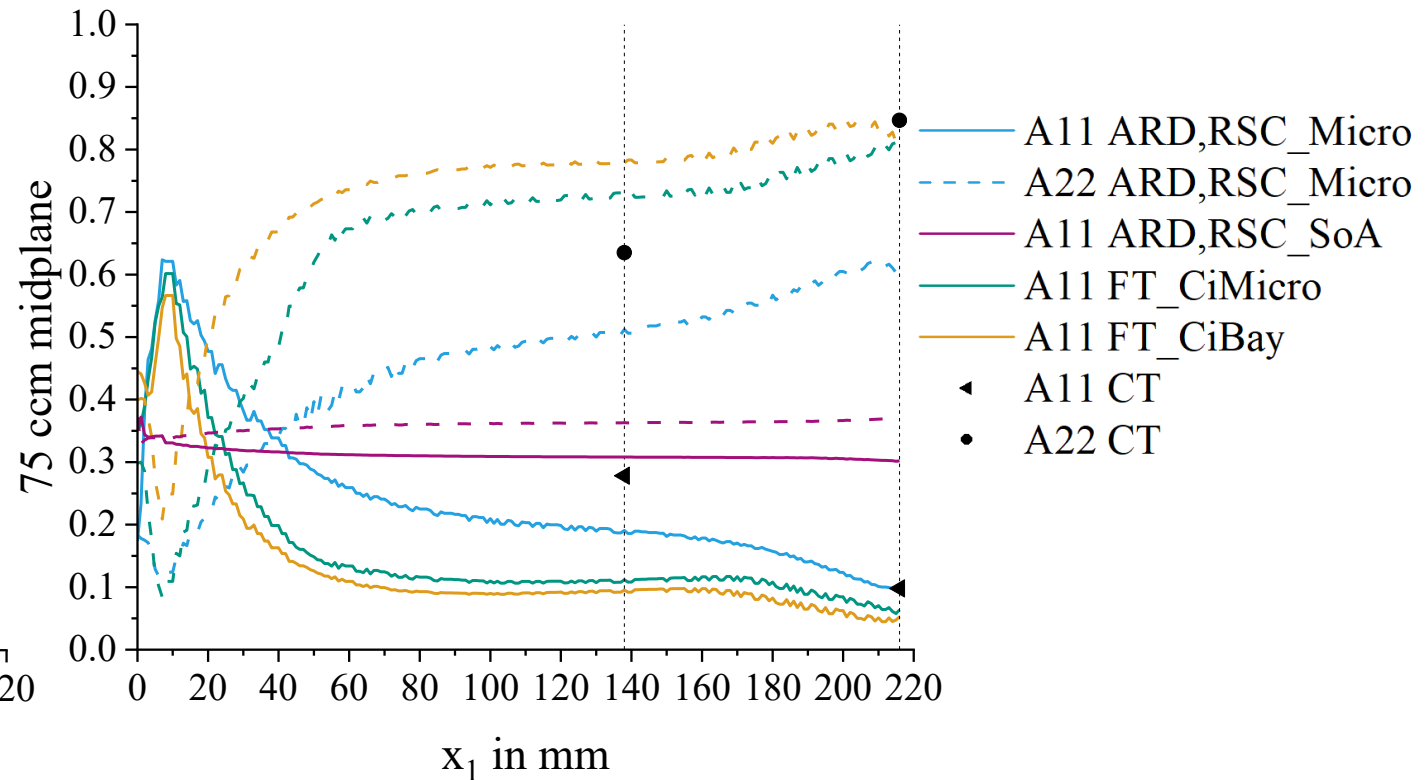
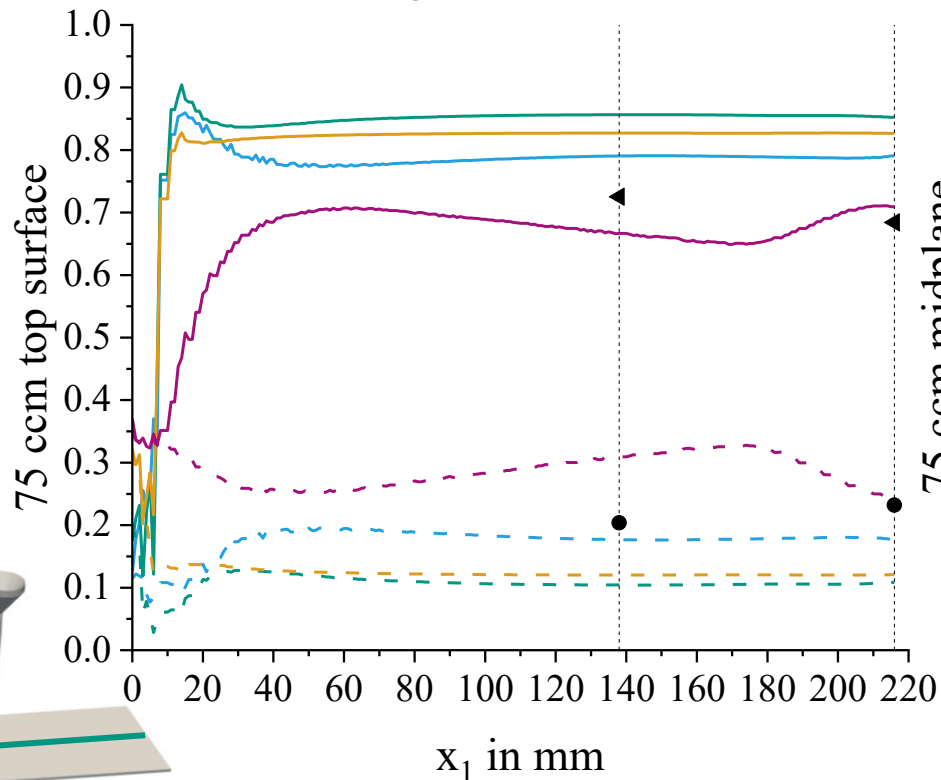


(Wittemann et al. 2025)

Macro-scale results

Parameter fitting

- Results for 75 cm³/s along the flow path
- Nearly no change in midplane for ARD-RSC with SoA parameters
- Fitted parameters show right tendencies in midplane



(Wittmann et al. 2025)

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Summary

- SPH based micro-scale model with individual fibres in Newtonian fluid
 - Flexible and interacting fibres
- Parametrization of ARD-RSC approach with micro-scale results
- Good agreement with experimental results
 - Partially better results compared to SoA parameters, partially worse
 - Fitted parameters predict tendencies visible in experiments also over time/flow path

Next steps:

- More efficient micro-scale model
- Extend to validation to other material systems, longer fibres and higher fibre volume content

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Thank you for your attention

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Groupleader Mold filling simulation

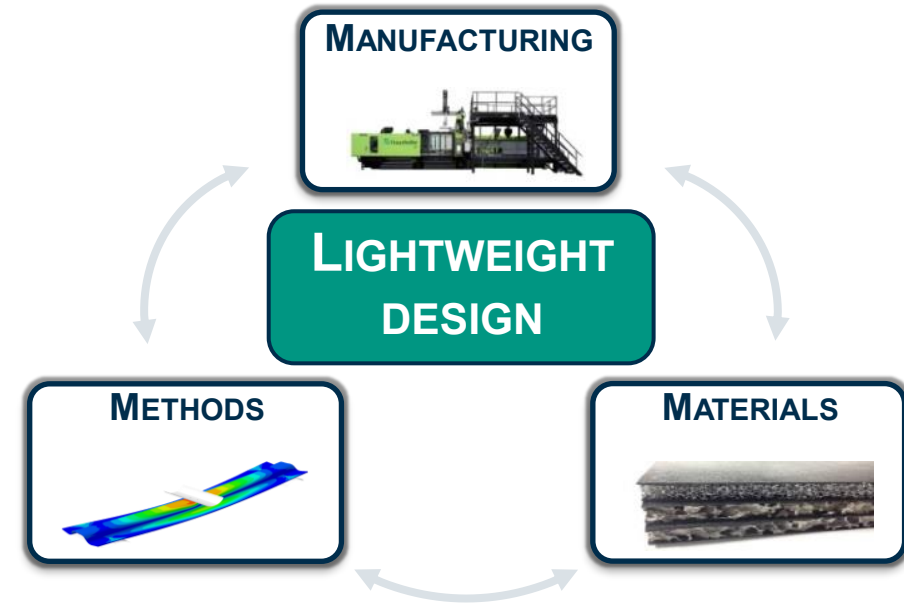
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Lightweight Design Network



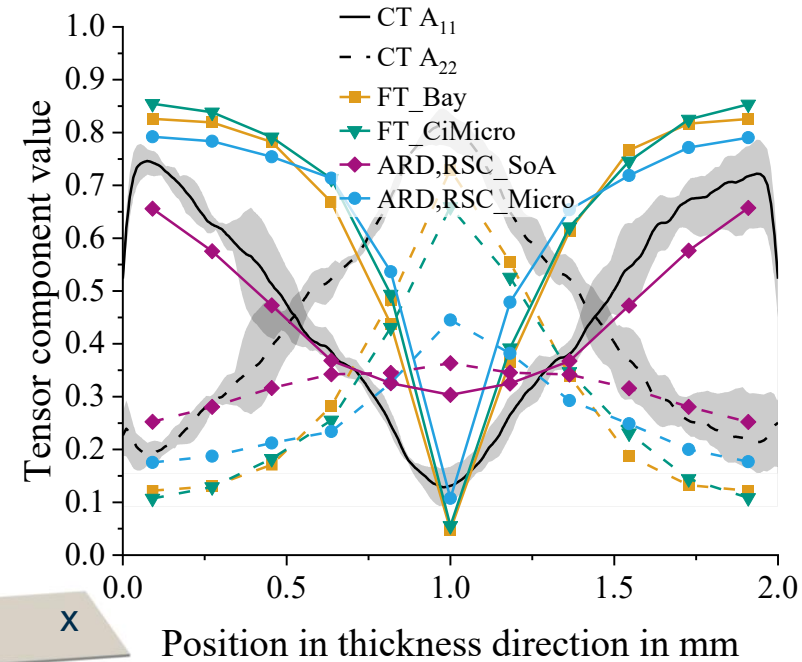
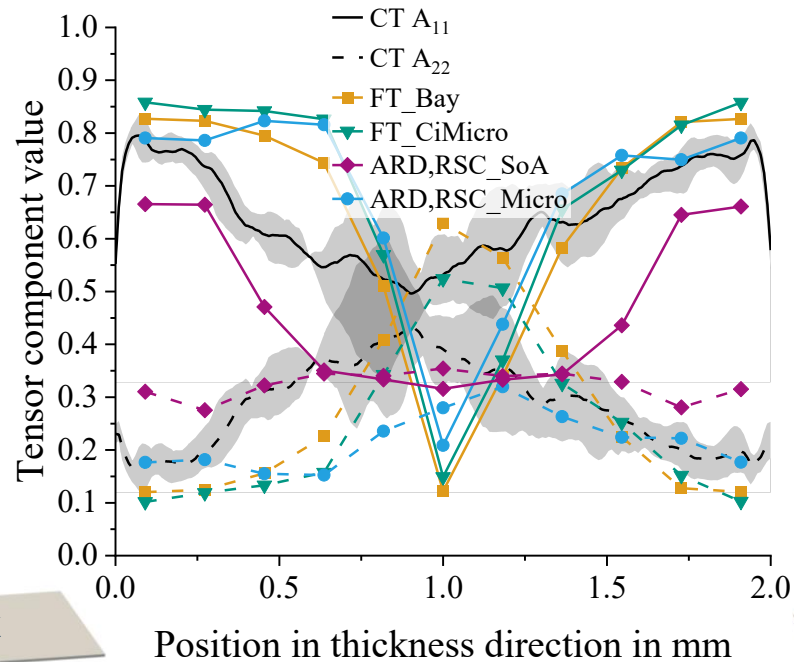
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Appendix

Results for 50 cm³/s

- Results for 50 cm³/s
- FT and fitted ARD-RSC are quite similar in A₁₁
- Clear difference between SoA and fitted parameters for ARD-RSC
- Fitted ARD-RSC fits best near the wall

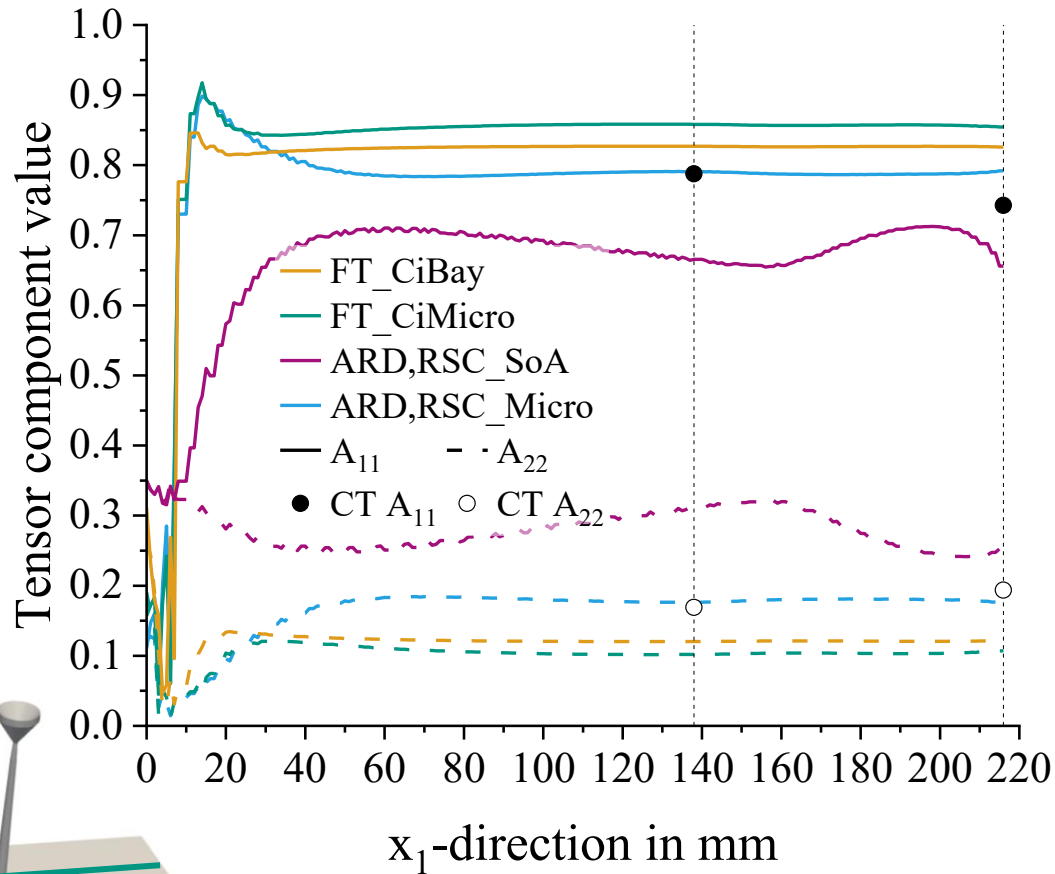


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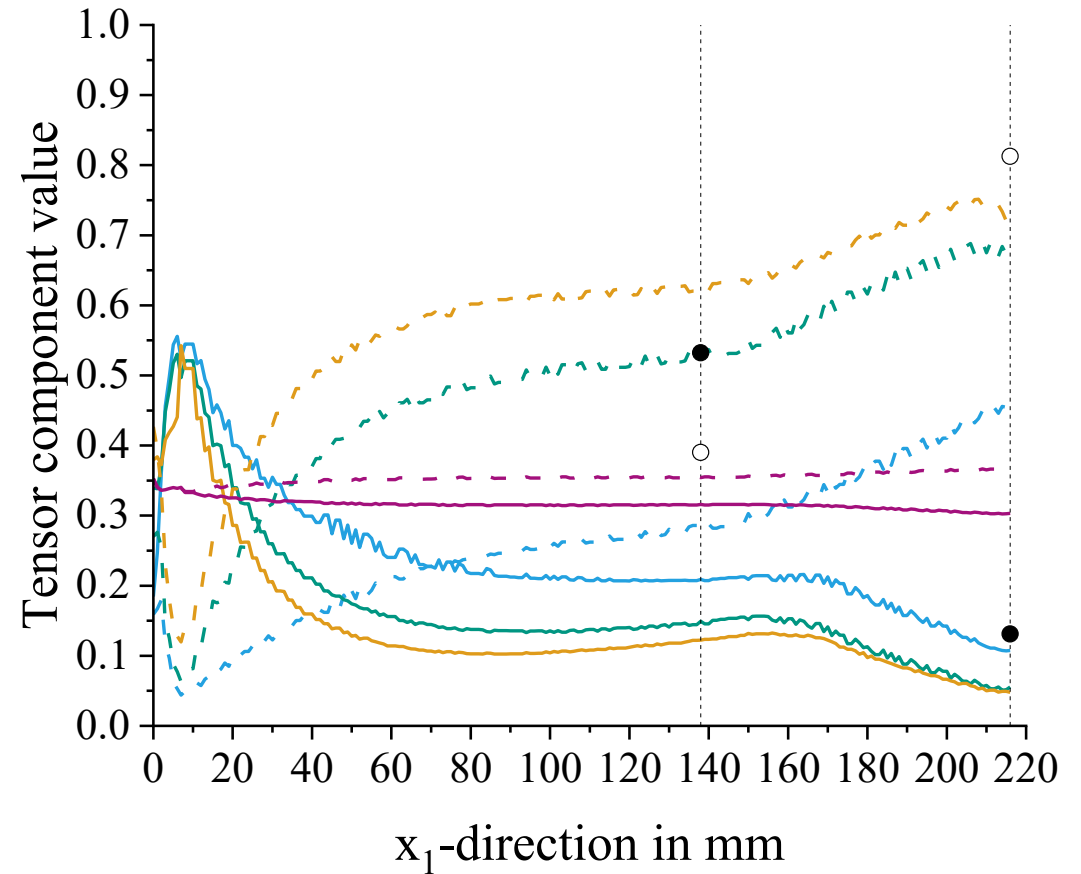
Appendix

Results for 50 cm³/s

- Results for 50 cm³/s along the flow path



(a)

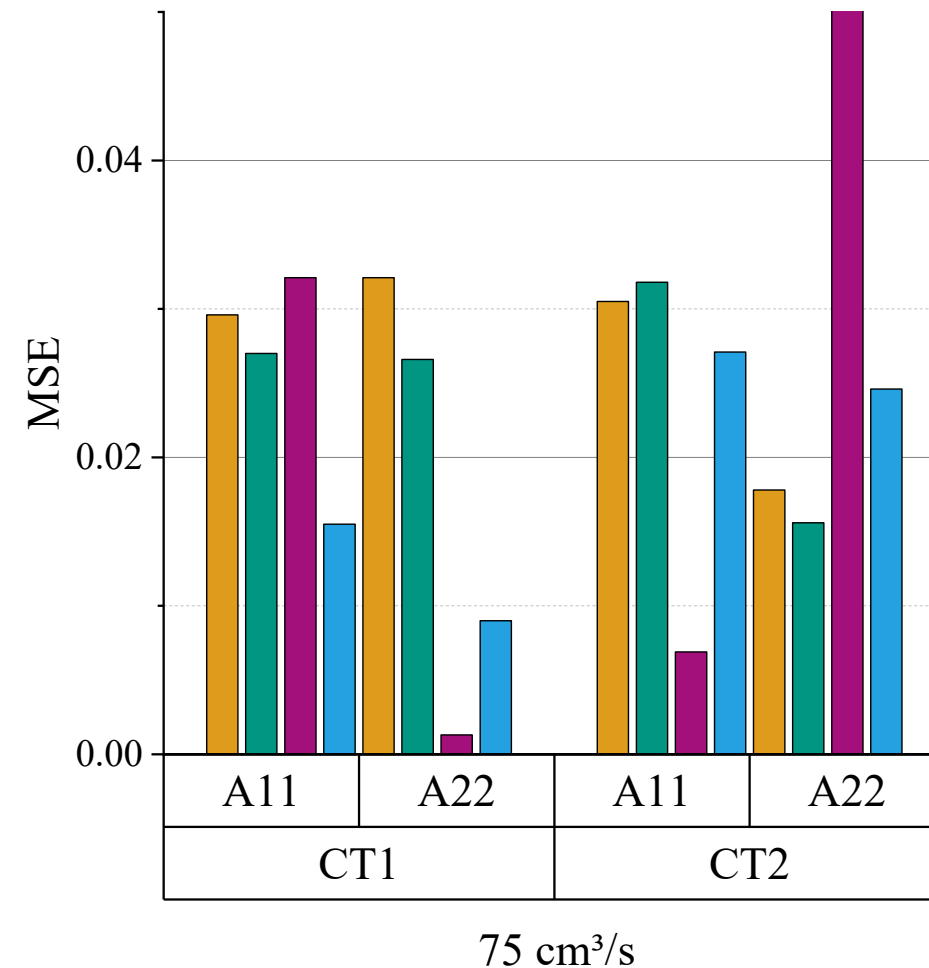
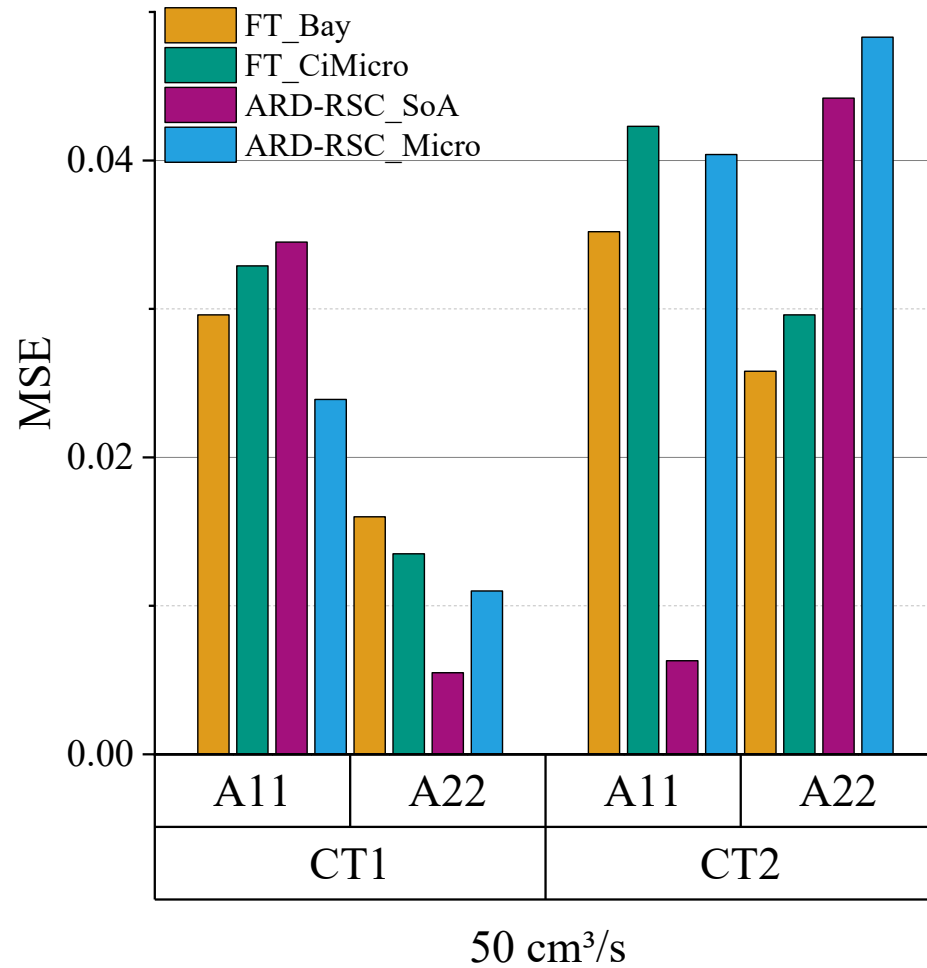


(b)

(Wittmann et al. 2025)

Appendix

MSE



(Wittmann et al. 2025)