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Micro-scale model for a multi-scale modeling approach of thermoplastic fiber reinforced polymers

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Abstract. Thermoplastic fiber reinforced composites (TPFRCs) are becoming more important due to the potential of short part cycle times and recyclability. One major problem of these materials is process stability. During processing, unwanted distortions appear due to residual stresses on different scales. The prediction of these distortions and stresses would reduce the cost of TPFRCs and would assist in achieving a higher market share. For the prediction of the residual stresses, a new multi-scale simulation approach is required. The research presented in this paper is a contribution to the micro-scale model. A method for the representation of the thermoplastic matrix in a 2D micro-scale model is developed. With this, the solid as well as a semi-liquid state of the polymer which appear during thermoforming can be represented.

1. Introduction

The demand for lightweight materials is rising due to resource scarcity and environmental awareness. Fiber reinforced polymers (FRPs) are among the strongest lightweight materials, which combine high mechanical properties with low density. The FRPs with the highest mechanical properties contain thermoset polymer matrices, which are cured irreversibly through a chemical reaction. Even though thermoplastic composites have inferior mechanical properties, they are becoming more popular due to the potential of shorter part production cycle times, ease of storage and handling, increased toughness and recyclability [1][2].

Thermoplastic fiber reinforced composites (TPFRCs) often come in the form of blanks which are processed by applying heat and pressure in a thermoforming process. Despite the short cycle times and easy handling, TPFRCs do not have a high market share, which is around ten percent [2]. One major issue for these materials is the process stability. Residual stresses occur due to several effects on different scales, which cause unwanted deformations [3]. Currently, attempts to mitigate unwanted residual stresses rely on trial and error, which can be cost intensive and time consuming [4].

Computational models of the thermoforming process which can predict shape distortions and residual stresses are needed to replace trial and error. A multi-scale approach is required due to the multi-scale nature of the residual stresses [1]. Typical scales for modeling of TPFRCs are micro-, meso- and macro-scale [1]. On the micro-scale, the discrete element method (DEM) will be utilized to include the solid as well as the semi-liquid state of the TPFRCs during the thermoforming process. For this, an existing code for the calculation of dry carbon fibers introduced in [5] will be expanded by adding a matrix, which is
temperature dependent. Thus, with the model contacts mechanics between single filaments will be represented. Additionally, the solid as well as the semi-liquid state of the matrix will be considered. For this, springs representing the matrix are implemented in the DEM model shown in [5]. These springs are dependent on geometrical and material property factors. With this, a temperature dependent material model will be developed and applied to the springs. The basic rules for the implementation of the matrix springs in the DEM model are explained in the following chapters.

2. Model description
The matrix model is based on springs with a stiffness dependent on the material properties and geometry factors. For this, an independent continuum mechanics model is created. The model calculates the forces for each fiber solely based on the matrix springs. For the application of these springs, rules to implement the matrix are developed. These rules are introduced hereinafter.

The model is based on two types of connections: fiber-fiber and fiber-matrix connections (Figure 1). These connections are meant to resemble the influence of the matrix on fibers. The fiber-fiber connection is used to represent the interaction between any two adjacent fibers. It is assumed that the two fibers are connected by a conical portion of the matrix. The fiber-matrix connection is used to represent interaction between fibers and matrix. These portions are attached to the given fiber, fiber \( i \) and to the portion of the matrix between any two of the neighboring fibers, fiber \( j \) and fiber \( k \). The exact point of the attachment for the fiber-matrix connection will be explained below. To establish any of these connections it is required to know the neighbors of a given fiber. The method used to find neighboring fibers for any of these fibers is presented in the following section.

![Figure 1](image_url)

**Figure 1.** a) Matrix portion between two fibers, b) matrix portion of a fiber and matrix without an adjacent fiber

2.1. Neighbor search
The connections must be established between appropriate fibers and must be attached to appropriate regions of the matrix. Thus, finding correct neighbors for each fiber is a crucial step. Neighbor selection is controlled by three parameters: search radius, maximum overlap angle and maximum relative fiber angle (Figure 2). The neighbor search for a given fiber starts with finding all fibers within the search radius. Next, all these fibers are sorted in ascending order with respect to the distance from the given fiber. After that, all sorted fibers, starting from the closest one, are checked. When a fiber is within the set conditions imposed by a maximum overlap angle and a minimum relative fiber angle, it is considered to be a neighbor of the given fiber. After finding the neighboring fibers the stiffness of the matrix portions need to be calculated, which is done in the following.
2.2. Stiffness Calculation

After all neighboring fibers are found, the stiffness of the matrix portions needs to be calculated. For this, the assumption is made, that each connection has solely normal stiffness in the direction of the connection. For now, all connections are assumed to be tapered rods made of linear elastic material under plane stress. Thus, normal stiffness of these connections can be found. The tangential displacements are assumed to be small compared to the normal displacement. Therefore, a tangential stiffness is not included in the calculation.

For the calculation of the matrix stiffness the geometry of the matrix is a key part. The geometry is approximated by a frustum shown in Figure 3. The frustum has the length $L$, the frustum angle $\theta$, a base height $h_0$ at the given fiber and the height $h_1$ at the neighboring fiber.

![Figure 2. Parameters considered in the neighbor search: a) edge overlap, b) relative fiber angle, c) search radius](image)

![Figure 3. Geometrical parameters used in stiffness calculation](image)

Considering the geometry, the frustum angle, $\theta$, can be found as

$$\sin \left( \frac{\theta}{2} \right) = \frac{r_{f1}}{l_f}$$

(1)
where $r_{f1}$ is the radius of the neighboring fiber and $l_f$ the length between the fiber centers. The given fiber side base height and the neighbor fiber base height are found as

$$h_0 = 2 \tan \left( \frac{\theta}{2} \right) r_{f0} \quad (2)$$

$$h_1 = 2 \tan \left( \frac{\theta}{2} \right) (l_f - r_{f1}) \quad (3)$$

To find the normal stiffness, the frustum was assumed to be rigidly fixed at the neighbor fiber’s side and loaded by an axial force at the given fiber’s side (Figure 4). The normal displacement of the frustum, $\delta_n$, is calculated as

$$\delta_n = \int_0^L \frac{F}{EA(x)} \, dx \quad (4)$$

where $F$ is the axial load, $E$ the Young’s modulus and $A(x)$ the area, which can be calculated with the height in dependence of the position $h(x)$ and the thickness $t$ as

$$A(x) = t \cdot h(x) \quad (5)$$

Assuming a general spring equation, the normal stiffness, $k_n$, can be calculated as

$$k_n = \frac{Et(h_1-h_0)}{\ln(h_1/h_0)L} \quad (6)$$

![Figure 4. Calculation model for the matrix stiffness](image)

2.3. Calculation of the fiber-matrix connections

The calculation of the stiffness $k_n$ for fiber-matrix connections is done equally as for the fiber-fiber connections. The geometric parameters are calculated in a different way, which is shown in Figure 5. The frustum angle $\theta$ is calculated by subtracting the angle between two fibers $\theta_{jk}$ by the half of each fiber’s angle $\theta_{ij}$ and $\theta_{ij}$. The position vector of the given fiber, fiber $i$ is $\mathbf{r}_{A0}$, the position vector of the neighboring fiber, fiber $j$ is $\mathbf{r}_{B0}$ and the position vector of the neighboring fiber, fiber $k$ is $\mathbf{r}_{C0}$. The position of the matrix between two fibers is described as $\mathbf{r}_{D0}$. The vector from the given fiber to the matrix position $\mathbf{r}_{D0}$ is $\mathbf{a}$.

$$\mathbf{r}_{D0} = \frac{\mathbf{r}_{A0} + \mathbf{r}_{C0}}{2} \quad (7)$$

$$\mathbf{a} = \mathbf{r}_{D0} - \mathbf{r}_{A0} \quad (8)$$

The length of the frustum is calculated with the radius of the given fiber $R_i$ and the positions of the matrix as

$$L = \|\mathbf{a}\| - R_i \quad (9)$$
With the length of the frustum and the angle between the fibers, the base height and the height can be found as

\[ h_0 = 2 \tan \left( \frac{\theta}{2} \right) R_i \]  
(10)

\[ h_1 = 2 \tan \left( \frac{\theta}{2} \right) L \]  
(11)

With the deformation for each connection, the forces acting on each fiber can be calculated.

**Figure 5.** Geometric parameters of fiber-matrix connections. a) angles between fibers, b) frustum between fibers

2.4. Calculation of the deformation

After the determination of the stiffnesses the deformations during one time step of the model need be calculated. To calculate the deformation, the given and its neighboring fiber are assumed to have initial positions \( \mathbf{r}_{E0} \) and \( \mathbf{r}_{B0} \) respectively. These positions define the initial configuration. During a load step the given fiber moves the distance \( u_A \), while the neighboring fiber moves the distance \( u_B \) (Figure 6).

**Figure 6.** Relative movement of fibers described with the fiber position vectors \( \mathbf{r}_{A0} \) and \( \mathbf{r}_{B0} \), the fiber displacements \( u_A \) and \( u_B \) and the relative fiber vectors \( \mathbf{a} \) and \( \mathbf{b} \).

The final positions after displacement can be calculated with the initial position \( \mathbf{r}_{B0} \) and \( \mathbf{r}_{B0} \), the displacement \( u_A \) and \( u_B \) and the relative fiber vectors \( \mathbf{a} \) and \( \mathbf{b} \). Finally, the change in length \( \Delta l_n \) of the connections can be calculated with the relative fiber vectors \( \mathbf{a} \) and \( \mathbf{b} \) as

\[ \Delta l_n = \| \mathbf{b} \| - \| \mathbf{a} \| \]  
(12)
2.5. Deformations of the fiber-matrix connections
For the calculation of the change in length at a fiber-matrix connection, three fibers are considered: The given fiber, fiber $i$ and the two neighboring fibers, fiber $j$ and fiber $k$ (Figure 7). The calculation is equal to the calculation of the fiber-fiber connection.

![Figure 7](image)

**Figure 7.** Relative movement of the fiber-matrix connection including the given fiber, fiber $i$ and the neighboring fibers, fiber $j$ and fiber $k$. The initial configuration is highlighted with solid lines, the configuration after displacement with dashed lines.

2.6. Calculation of the forces
For the connections between a given fiber and its neighboring fibers (Figure 8), there are two types of connections: Fiber-fiber connections established between the given fiber and its neighboring fibers (Figure 8 a), and fiber-matrix connections established between the given fiber and the middle portion of the matrix between two of the neighboring fibers (Figure 8 b). The middle portion of the matrix between two of the neighboring fibers is also connected to the neighboring fibers with a rigid rod (Figure 8 c).

![Figure 8](image)

**Figure 8.** Connection types: a) fiber-fiber connections, b) fiber-matrix connection, c) matrix to fiber rod connection.

Forces acting on the given fiber are calculated in the deformed configuration. Deformations and directions of all connections relevant to the given fiber are calculated. With stiffness, deformations and directions of all direct and indirect connections, the resulting force acting on the given fiber can be calculated.

Before the calculation of the forces acting on fibers, all connections and stiffnesses of the connections are defined. To calculate reaction forces acting on a given fiber, all connections relevant to the fiber should be found. In Figure 9 all relevant connections for a given fiber example are shown. The next step is to calculate the deformation of each connection, which is done as explained in the previous sections. The forces can be calculated with $F_{\text{con}} = (\Delta \ell_n \cdot k_n) \cdot \vec{F}_n$, whereas $F_{\text{con}}$ is the connection force for the
connection \( n \), \( \Delta l_n \) the change in length of the connection \( n \), \( k_n \) the stiffness of connection \( n \) and \( \hat{n}_n \) the unit vector which defines the direction of the connection \( n \).

![Diagram of force directions](image)

**Figure 9.** Force directions of: a) Fiber-fiber connections, b) fiber-matrix connection and c) indirect fiber-matrix connections.

3. Validation
The validation of the reduced spring model is done by comparing the reduced model to an equal FE model created in Abaqus unified FEA from Dassault Systèmes, Vélizy-Villacoublay, France. [6] This is done for a model a size of 0.4 mm times 0.4 mm in which the fiber radius is 0.01 mm. The search radius for neighbors was determined with a convergence study which is shown in Figure 10 and set to eight times the fiber radius (0.08 mm).

![Diagram of search radius convergence](image)

**Figure 10.** Search radius convergence study
The maximum edge overlap angle was set to 5° and the minimum relative fiber angle was set to 25°. With this configuration, all neighboring fibers for both models were sufficiently found. Two different approximated volume fractions were studied: 20 % and 48 %. At the top and bottom edge, the fibers were arranged in a row with a small gap of 5 % of the fiber radius to apply boundary conditions. The bottom row was fixed in all directions and at the top row the deformation was applied. The other fibers were distributed at random positions within the model. A comparison of the reduced model with FE model is shown in Figure 11 a) and b). The material parameters for both calculations as well as the specific FE model parameters are shown in Table 1.

| Table 1. Simulation parameters |
|--------------------------------|
| Matrix Young’s modulus        | 2000 MPa                  |
| Matrix Poisson’s ratio        | 0.3                       |
| Fiber Young’s modulus         | 73000 MPa                 |
| Fiber Poisson’s ratio         | 0.22                      |
| Mesh size                     | 0.001 mm                  |
| Element type                  | CPE4R                     |
| Step                          | Nonlinear static          |

The first validation is done with a tensile displacement simulation. For this, the top row of fibers was moved by 0.01 mm in the y-direction and fixed in the x-direction. A comparison of the undeformed and the deformed model is shown in Figure 11 c) and d). For each volume fraction, three different random fiber distributions are used for calculation. The reaction forces in loading direction of both models for each random fiber distribution are shown in Figure 12.

**Figure 11.** Comparison of the FE model a) and the reduced model b) for a low volume fraction and comparison of the undeformed c) and deformed d) model for a higher volume fraction
The reaction forces predicted by the reduced model in the direction of deformation are close to the reaction forces calculated with the FE model. The forces in x-direction are insignificantly small and therefore not discussed anymore. The standard deviation of the different random distributions is smaller than 1 % difference. The mean results of the model are within 10 % deviation from the FE model results.

The second validation is a compression loading simulation. For this, the top row of fibers is moved by 0.01 mm in negative y-direction and fixed in x-direction. The reaction forces in loading direction of the bottom row are shown in Figure 13.

The third validation is a shear loading simulation. For this, the top row of fibers is moved by 0.01 mm in positive x-direction and fixed in y-direction. The reaction forces in x-direction of the bottom row are shown in Figure 14.
The reaction forces predicted by the reduced model for the shear load are close to the reaction forces in FE model. The forces in y-direction are insignificantly small and therefore not discussed anymore. The standard deviation of different random distributions is less than 10% difference. The mean results of the model are within 10% deviation from the FE model results.

4. Conclusions
In summary, a matrix model for a 2D micro-scale simulation is introduced. The reduced model is dependent on material properties as well as geometrical factors. With these, neighboring fibers are identified and two different types of connections are established: fiber-fiber and fiber-matrix connections. With this discretization, any material model (e.g. one which is more accurate and temperature dependent) can be implemented in the micro-scale model.

For the validation, the reduced model is compared to an equivalent FE model. Different calculations are carried out. The results are within a 10% difference of the reduced model and the FE model for the tension and shear loading and within 15% difference for the compression loading. It can be concluded that the model approach for the matrix fit the FE model results sufficiently. Therefore, the matrix can be integrated in the fiber model presented in [5]. After the integration and testing of this solid configuration, a matrix in semi liquid state needs to be observed. This can be done by lowering the material properties. Finally, an adequate material model for the thermoplastic matrix will be introduced for the calculations.

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