ABSTRACT

The purpose of this research is to elaborate a mathematical model that describes the visco-elastic bending behavior of a thermoplastic composite specimen during thermoforming processes. The mathematical model was derived from a simplified physical model which represents a layered composite material of alternating elastic and viscous layers. In a previous research the viscous layers are assumed to be from Newtonian fluid, having a constant shear viscosity, while the elastic layers are linear elastic. This resulted in a mathematical model in form of the diffusion equation, describing a diffusive-like behavior of the deflection angles in the beam. Because polymeric melts exhibit in general a shear thinning behavior, the diffusion equation in this research is improved by including the shear rate dependency of the melt viscosity. Therefore, the diffusion equation became a non-linear differential equation, which is solved numerically by means of the finite difference method. This research shows the significance of the shear thinning behavior in the model by comparing the bending deformation of the composite beam obtained with a constant viscosity and a shear-thinning viscosity.

ACKNOWLEDGEMENTS

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I would like to thank Remko Akkerman for helping me find this assignment and introducing me to thermoplastic composites. The challenging discussions and the good feedback has helped me a lot in the understanding of the problem and the context around it. I also would like to give a great thanks to Ulrich Sachs, we had a great cooperation and you were always there when I needed help. Your readiness to help me out and send me in the right direction where a great help.

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1 INTRODUCTION

Climate change has become over the years a popular subject. People are nowadays more aware of the consequences of our current life style. Creating an ecofriendly society has become a more important item on the agenda for more governments. In June 2015, the Dutch government has received the verdict that it has to reduce the greenhouse gas CO2 with 25% in 2020 [1].
At the same time, society is not willing to pay huge amounts extra or reduce their luxury in order to help this cause. This creates a large challenge and has caused researchers to search for alternatives, which are cheap, can provide luxury and lower emissions.

The ThermoPlastic composite Research Center (TPRC) is one of the places where researchers are doing research into a new material. This material, thermoplastic composites, can replace the current building materials in the automotive and aerospace industry. It is a lighter alternative and lighter vehicles have a lower emission rate. As an added bonus, thermoplastic composites also form a tougher and stronger material [2].

At this moment, the thermoset composites are often used even though thermoplastic composites have a higher toughness and impact damage resistance [2]. The reason for this is that thermoset composites have lower material costs [3]. However they are less suitable for automated processes and the products are mainly made by hand lay-up. Thermoplastic composite are more suitable for production processes, because of the melting property of thermoplastics. However the behavior of thermoplastic composites in a forming process is complicated. Currently there is a lag in knowledge about their behavior, which prevents the material from becoming popular in use. [3]

When this knowledge gap has been bridged, the thermoplastic composites will play a larger role in the automotive and aerospace industry. Apart from being tougher and less prone to damage, thermoplastic composites also have the property of being recyclable. Production will be a lot cheaper as well, due to the fact that thermoplastics are easier to handle in forming processes.

Currently the TPRC, together with BOEING, Fokker, Ten Cate and the University of Twente, is doing research to close the knowledge gap in the behavior of this material. This is done by predicting the behavior of the thermoplastic composites in different production operations.
In this paper the bending of a thermoplastic composite will be discussed. By predicting the behavior of the composite during the bending process, the reluctance of the material to bend can be determined. With this information, the bending process can be optimized to prevent formability problems.

Currently there is a model on the behavior of the composite during the bending process.
This model is however very simplified. In this report the model will be elaborated.

2 THEORETICAL BACKGROUND

2.1 Thermoplastic composites

In order to predict the bending behavior, the structure of a thermoplastic composites is essential. A composite material is a material that consists of a stack of multiple materials. These materials keep their own material properties, but put together other characteristics appear. In the case of thermoplastic composites, it is a stack of alternating layers of fiber (e.g. glass fiber) and thermoplastic polymers. The fiber layer can have a woven structure of polymers or a unidirectional (UD) structure, see figure 1. UD composites are for production and stiffness reasons more beneficial, however it does cause more problems when bending the material [2]. This research considers the UD fiber reinforced polymers in the thermoplastic layer of the composite.

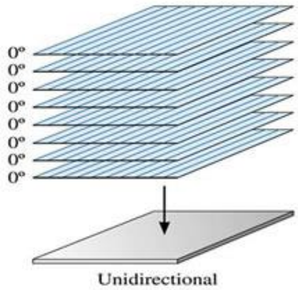

FIGURE 1: UNIDIRECTION COMPOSITES [5]

Thermoplastics, also known as thermosoftening plastics, are a type of material that consists of long polymer chains (figure 2). Thermosoftening plastics melt when temperature is increased and harden out when the temperature is lowered again. This explains why this material is easy to produce and is suited very well for recycling

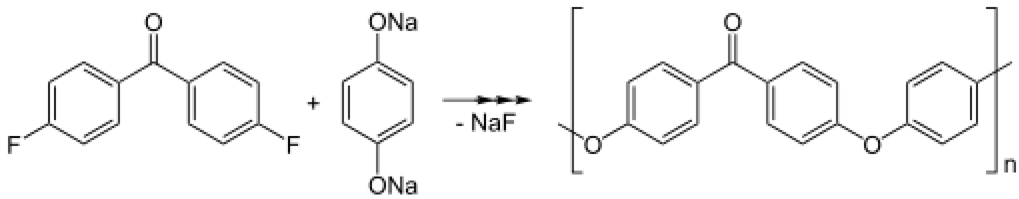

FIGURE 2: POLYETHERETHERKETONE (PEEK) [6]

2.2 Bending in forming processes

In the bending process, the material must not lose any of its strength and toughness. This is prevented by heating the composite above melting temperature of the thermoplastic during the bending process. When the bending process is completed, the specimen is cooled down. This process prevents the composite from having to bend in the solid phase, which would cause stress on the polymers. Instead the polymer layer is able to form in the molten phase, resulting in having the same toughness as before can be achieved if it is well consolidated.

2.3 Bending experiment

The bending of a thermoplastic composite is done with the use of a rheometer. The rheometer has a thermal chamber which will heat up the specimen above melting temperature. When the chamber is at the right temperature, the specimen will be clamped in the two fixtures as can be seen in figure 3. One fixture stays at a zero degree angle (the reference angle) and the second fixture will rotate around the shaft at a constant velocity (ω).
To rotate and therefore bend the specimen, a certain amount of moment (M_c) has to be exerted by the rotating shaft. This moment is dependent on the amount of resisitance the specimen has to bend. The rheometer can measure the moment exerted on the shaft and thus measuring the reluctance of the specimen to bend.

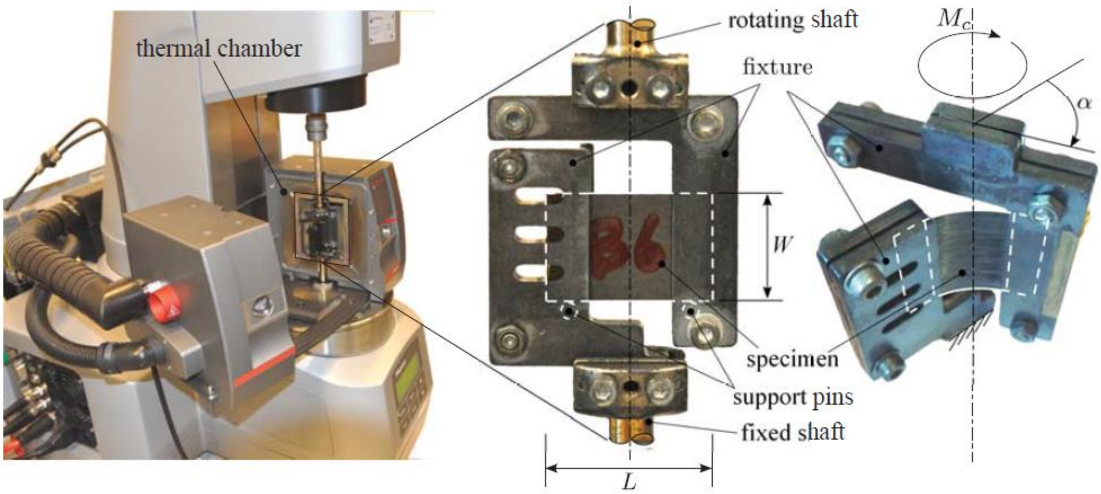

FIGURE 3: RHEOMETER USED IN RESEARCH U. SACHS [2]

2.4 Bending model

To predict the behavior of the specimen during the experiment a model is made. In order to make a feasible model the following simplifications are made:

- The fibers and matrix are evenly distributed.
- The fibers and matrix are modeled as layers with a homogeneous thickness, h_f and h_m, respectively.

Now that the model is simplified, the forces and moments can be considered.
The specimen will bend due to the moment M put upon the end. This moment will only bend the fiber layers - the matrix layers cannot carry moments, due to their melted phase. The fiber layer will also experience a transverse force V and a normal force N as a result of the fixtures.
Due to the fact that the laminate is a stack of fiber layers (alternated with matrix layers), the separate layers bend separate of each other. As a result they slide relative to each other, figure 4. This sliding will result in a relative shear force. A shear force is a force that in the direction of the slide, it will try to deform the material it is being exerted on. The shear force caused by the sliding of the fiber layers is related to the height of the matrix layer and the size of the step looked into. This has to do with the viscosity of the matrix layer, if the layer is really thin the shear force should be larger to make the deformation (by sliding the fiber layer). The force is also linear to

the size of the step $\frac{Q}{h_m} \cdot ds$. The shear force perpendicular to the layer is the non-proportional shear force in the layer. The forces and moments on the layers are displayed in figure 4.

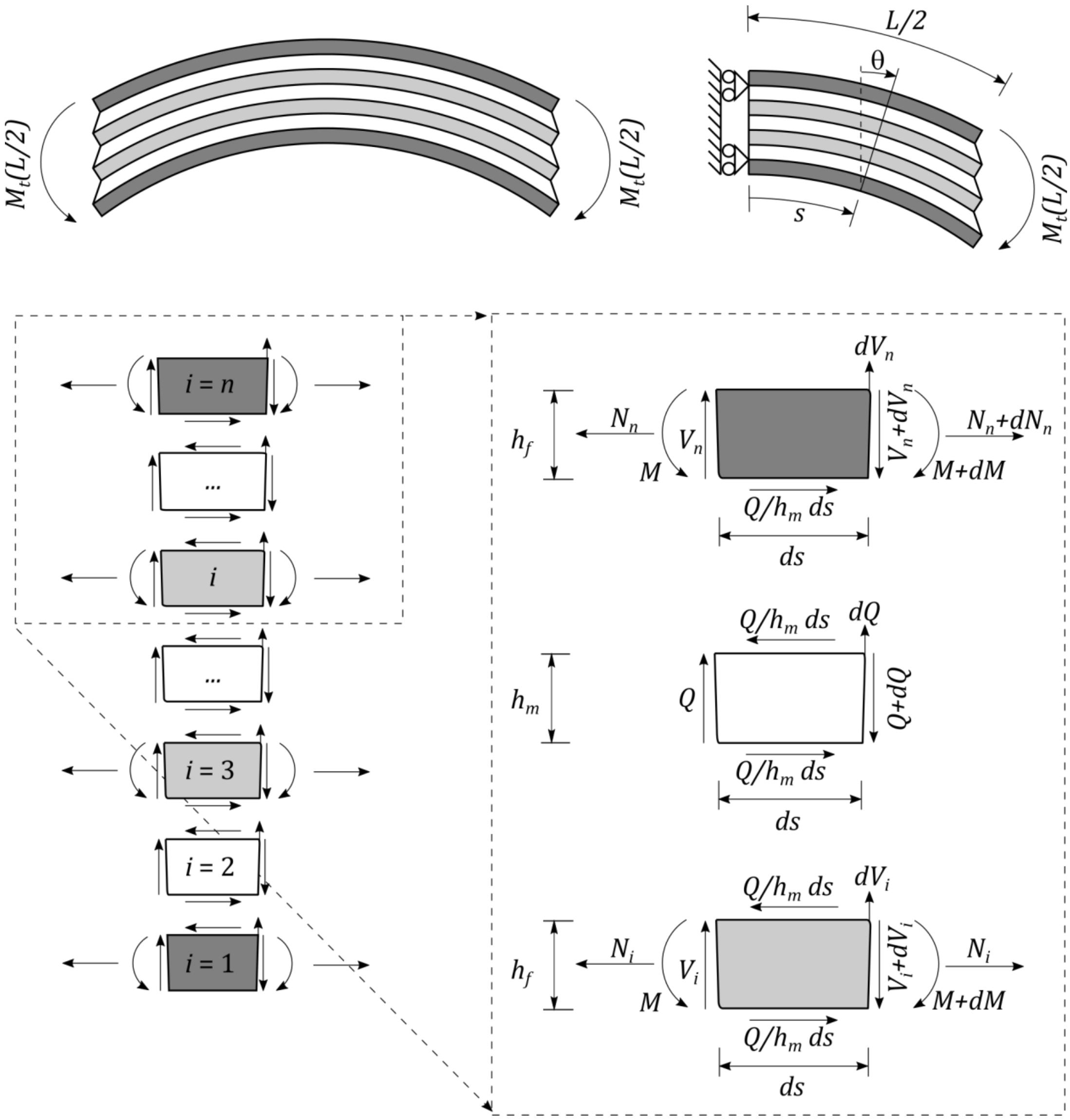

FIGURE 4: BENDING OF COMPONENTS SHACKED

2.5 Assumptions for the mathematical model

To make a mathematical model for this specimen, assumptions have to be made.

- The thickness of the laminate H is small in comparison to the bending radius ρ: $\frac{H}{\rho} \ll 1$.
- This implies that: $ds \approx ds_i$, where i is the layer index.
- The matrix layer can only carry shear forces.
- The fiber layer deform due to bending moments.
- The matrix is a Newtonian viscous fluid with viscosity η.

- The fiber is a Hookian elastic solid with elastic modulus E.
- The deformation of the laminate is considered small. Thus neglecting non-linearity by deformation.
- All fiber layers deform equally: $M = M_i$ and $dM = dM_i, \forall i$.
- All matrix layers deform equally: $Q = Q_i$ and $dQ = dQ_i, \forall i$.

2.6 Deriving the mathematical model

To derive the mathematical model, the magnitude of the shear force has to be defined. In the work of Sachs the definition was formed for the shear γ of a thermoplastic composite as a function of the deflection angle θ [2]. This relation is based on the fundaments of the azimuthal strain (strain in a bending situation) of a single layer. Since h_f and h_m are independent on time, the time derivative of shear, the shear rate $\dot{\gamma}$, is therefore in the same way related to the rate of deflection angle $\dot{\theta}$.

$$\gamma = \left(\frac{h_f}{h_m} + 1\right) \theta \qquad \textbf{1.}$$

This relation is combined with the definition of the shear force with W as the width of the specimen. Since h_f and h_m are independent on time, the time differentiable of shear, the shear rate, is therefore in the same way related to the rate of deflection angle.

$$Q = \eta \frac{\partial \gamma}{\partial t} h_m W = \eta \left(\frac{h_f}{h_m} + 1\right) \dot{\theta}\, h_m W \qquad \textbf{2.}$$

Now that the shear force is defined, the moment equilibrium has to be determined for a fiber unit cell embedded by matrix, $in \in \{3, 5, 7, \dots, n-2\}$:

$$dM + V_{in}\, ds - Q \frac{h_f}{h_m} ds = 0. \qquad \textbf{3.}$$

The moment equilibrium for a fiber unit cell on the outer surface, $out \in \{1, n\}$:

$$dM + V_{out}\, ds - Q \frac{1}{2} \frac{h_f}{h_m} ds = 0. \qquad \textbf{4.}$$

By subtracting equation 4 from equation 3 the following relation between the transverse forces and the shear force is determined.

$$V_{in} = V_{out} + Q \frac{1}{2} \frac{h_f}{h_m}. \qquad \textbf{5.}$$

A force equilibrium considering all n layers yields:

$$\frac{n-3}{2}\, dV_{in} + 2 dV_{out} = -\frac{n-1}{2} dQ. \qquad \textbf{6.}$$

Equation 6 is integrated from $s = 0$ till $s = L$. Since the shear force and the transverse force are zero at $s = 0$, forces are considered at $s = L$ and the equation simplifies:

$$\frac{n-3}{2} V_{in} + 2V_{out} = -\frac{n-1}{2} Q. \qquad \textbf{7.}$$

Solving with equation 5 for V_{out}:

$$V_{out} = -\left(\frac{n-1}{n+1} + \frac{1}{2}\frac{n-3}{n+1}\frac{h_f}{h_m}\right) Q \qquad \textbf{8.}$$

Assuming $n \gg 1$:

$$V_{out} \approx -\left(1 + \frac{1}{2}\frac{h_f}{h_m}\right) Q \qquad \textbf{9.}$$

Solving for V_{in}:

$$V_{in} = -\left(\frac{n-1}{n+1} - \frac{h_f}{h_m}\frac{2}{n+1}\right) Q \qquad \textbf{10.}$$

Assuming $n \gg 1$:

$$V_{in} = -Q \qquad \textbf{11.}$$

The final differential equation is based on the moment equilibrium of a fiber unit cell embedded in the matrix:

$$dM + V_{in}\, ds - Q\frac{h_f}{h_m} ds = 0 \qquad \textbf{12.}$$

$$\frac{\partial M}{\partial s} - \left(1 + \frac{h_f}{h_m}\right) Q = 0 \qquad \textbf{13.}$$

The moment in the fiber is related to its curvature according to the Euler-Bernoulli beam theorem, with I as the second moment of area of the fiber layer:

$$M = \frac{\partial \theta}{\partial s} EI. \qquad \textbf{14.}$$

Substitution of M and Q by the constitutive equations, will result in a partial differential, diffusion, equation.

$$D\frac{\partial^2 \theta}{\partial s^2} - \frac{\partial \theta}{\partial t} = 0 \qquad \textbf{15.}$$

$$D = \frac{EI_f}{\eta\left(1 + \frac{h_f}{h_m}\right)(h_f + h_m)W} \qquad \textbf{16.}$$

2.7 Boundary conditions

In order to solve the partial differential equation, boundary conditions are necessary. Boundary conditions describe the deflections already known. In this set of equations there are three different boundary conditions given, in which N represent the amount of space steps, ω the angular velocity of the fixture and Δt the size of the time step.

1. At time $j = 0$, the specimen is flat: $\theta_{i,0} = 0 \; \forall \; i$.
2. At space step $i = 1$, the specimen will not deflect: $\theta_{1,j} = 0 \; \forall \; j$.
3. At space step $i = N$, the specimen has the same angle of the fixture: $\theta_{N,j}(j) = \frac{\omega}{2} \cdot j \cdot \Delta t \; \forall \; j$. With ω as the angular velocity of the fixture.

2.8 Solution mathematical model

In figure 5 the solution of this diffusion equation is displayed, considering a specimen with a length of 7.5 mm, an angular velocity of the fixure $\omega = \frac{\pi}{3}$ and a diffusion coefficient $D = 7.7908 \cdot 10^{-7}$.

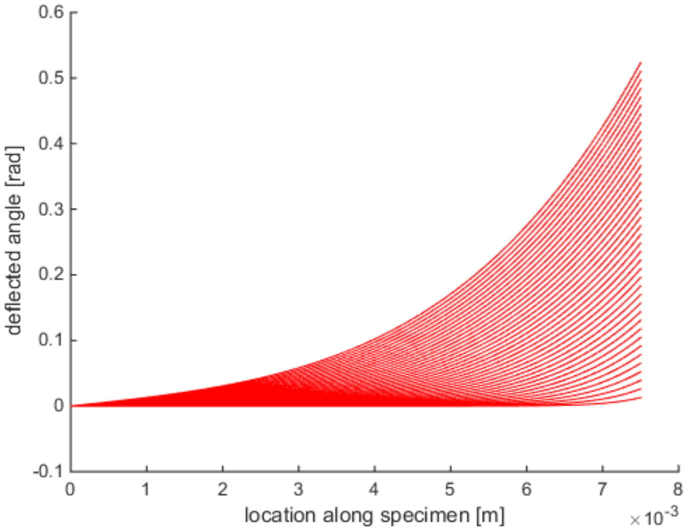

FIGURE 5: THE SOLUTION OF THE DIFFUSION EQUATION WITH A CONSTANT VISCOSITY OF 7.7908E-7

Equation 15 can be recognized as the diffusion equation in which D represents the diffusion coefficient or diffusivity. The diffusion coefficient indicates the rate of the diffusion. In this case the diffusion coefficient is dependent on the bending stiffness, the width of the specimen and the height of both the fiber layer and the matrix layer.

When the diffusion coefficient is infinite the local deflection angle moves instantly and linear throughout the whole specimen. At a diffusion coefficient approaching zero (e.g. $1 \cdot 10^{-15}$), the specimen is very reluctant to the given angle, and will stay straight as long as possible. The final deflection angle along the specimen for different values of the diffusion coefficient can be seen in figure 6.

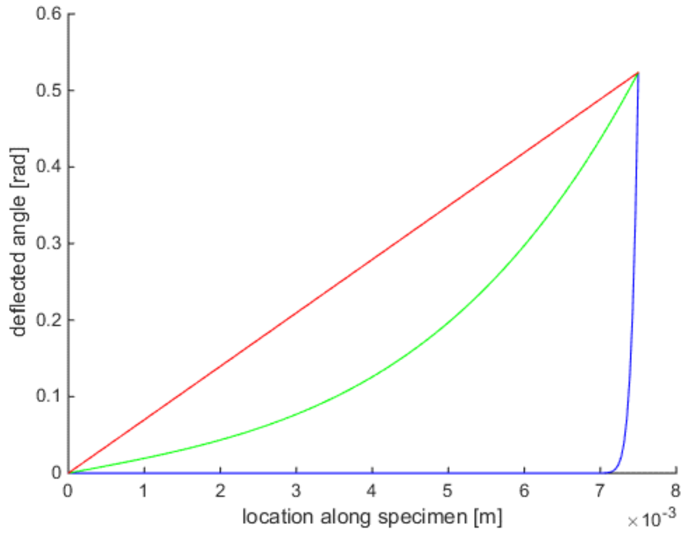

FIGURE 6: SOLUTION OF THE DIFFUSION EQUATION WITH IN RED D=1E15, IN GREEN D=1E-5, IN BLUE D=1E-8

2.9 Non-Newtonian fluids

When the old model is made, it was assumed that the viscosity of the matrix layer is constant. This assumption is however not true. During the bending process the thermoplastic layer is a molten phase. When looking at the viscosity of a thermoplastic melt, it can be observed that the viscosity is dependent on the shear rate [7]. This phenomenon is called the viscosity of a non-Newtonian fluid.

There are three big categories of viscosities for non-Newtonian fluids [8]:

- Viscoelastic viscosity, a combination of elastic and viscous effects, e.g. whipped cream.
- Time dependent viscosity, the viscosity either increases or decreases with the duration of stress, e.g. printer ink or yogurt
- Time independent viscosity, the viscosity is either increasing or decreasing with increased stress, e.g. suspensions of cornstarch in water or blood.

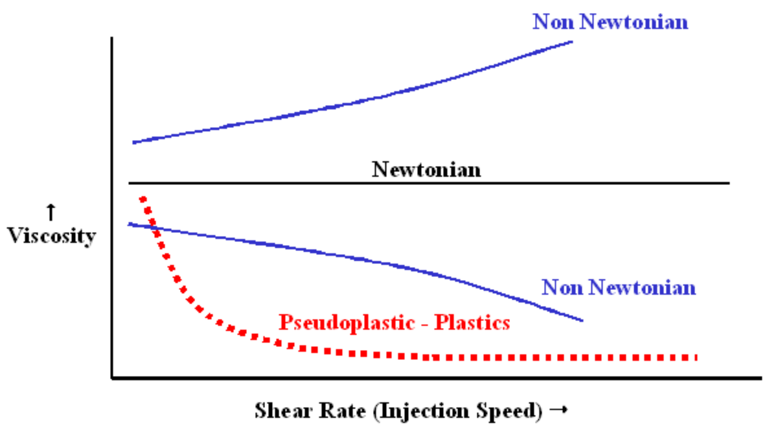

FIGURE 7: RELATION BETWEEN THE SHEAR RATE [1/S] AND VISCOSITY [PA.S] FOR DIFFERENT TYPES OF FLUIDS [9]

Thermoplastics often exhibit a shear thinning behavior, which decreases with an increasing shear rate. Shear rate is the rate at which a progressive shearing deformation is applied to the material [10]. Since the diffusion coefficient is inversely proportional to the viscosity, the diffusion coefficient increases when the shear rate increases.

The shear rate dependent viscosity for UD carbon PEEK was investigated by several researches done by different institutes, including the University of Twente [2] [11] [12]. When displayed in a logarithmic graph a clear relation between the viscosity and the shear rate can be seen in figure 7.

$$\eta = K\,\dot{\gamma}^{m} \qquad \textbf{17.}$$

The constants however are not exactly the same for the different experiments even though the same polymer is used. This difference can be explained by the different temperatures at which the experiments are done or the different grade of polymer used [7]. But it is very likely, that the measuring methods are different for each researcher. Therefore only speculation can be made from this data. These speculations have to be tested experimentally by using the same measuring methods with different conditions.

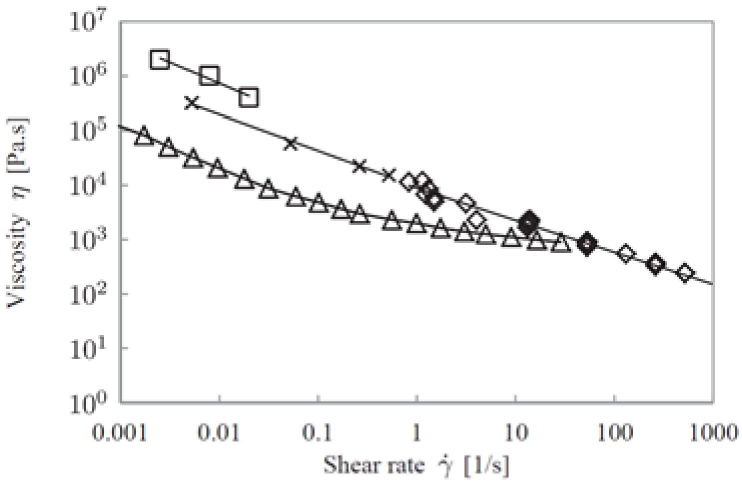

FIGURE 8: RELATION VISCOSITY AND SHEAR STRESS. × SACHS *ET AL* (UD CARBON PEEK AT 385°C); □ STANLEY AND MALLON (APC-2 AT 380°C); ◊ SACHS *ET AL.* (UD CARBON PEEK AT 390°C); Δ GROVES (UD CARBON PEEK AT °C) [2]

With the relation between the viscosity and the shear rate, the diffusion equation can be updated. The diffusion coefficient is dependent on the shear rate.

This result can also be verified with the measurements of the exerted moment on the shaft during the bending process. If the relation was purely visco-elastic, there would be a linear relation between the moment and the angle. As can be seen in figure 9, the relation is not linear. At low angles the moment is small, then the relation between the rotation angle and the moment are almost linear, up to the point when the angle is above approximately 50º.

In figure 9, the moment is measured at different angular velocities ($\dot{\alpha}$). A higher velocity would logically cause a higher shear rate, thus resulting in different values for the viscosity and the diffusion coefficient [2].

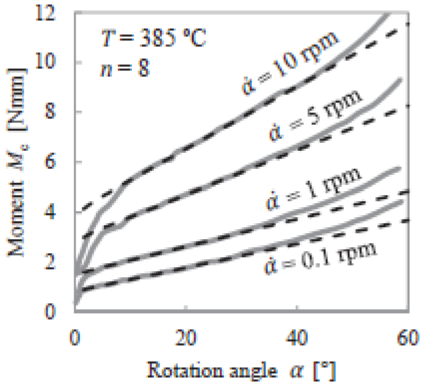

FIGURE 9: THE MOMENT THAT IS EXERTED ON THE SHAFT VS THE ANGLE OF THE BENDING FIXTURE, THE DOTT\
ED LINES REPRESENT THE FITTED MODEL OF SACHS.

3 METHOD

3.1 Finite Difference Method

When solving non-linear differential equations, like the diffusion equation with a shear rate dependent diffusion coefficient, an analytical approach is not always possible. Therefore the equation is solved numerically by using the finite difference method.

In this method the differential equations are converted into difference equations. These difference equations give an approximate of the first and second derivative at numerous points of interest. When this is done with infinitively many points an exact solution is established. However this is not possible and a finite number of points can give a fairly good solution as well. The amount of steps is inversely proportional to the step size. When the step size is small relative to the distance, the finite difference method gives a good estimate.

The two equations below represent the ways in which a first derivative and a second derivative are translated to the finite difference method. In this case the diffusion equation is being solved. The diffusion equation (equation 15) has the property that it contains the first derivative of time and the second derivative in space. i is the index of the space step and j is the index of the time step. Δs and Δt represent respectively the size of the space step and the size of the time step.

$$D\,\frac{\theta_{i+1,j} - 2\theta_{i,j} + \theta_{i-1,j}}{\Delta s^2} - \frac{\theta_{i,j+1} - \theta_{i,j-1}}{2\Delta t} \approx 0 \qquad \textbf{18.}$$

In this equation data are used both from a previous time step and one in the future, which gives complications when solving diffusion equations. Therefore a slightly less accurate translations must be used, considering only 2 different time steps.

$$\frac{\partial\theta}{\partial t} = \frac{\theta_{i,j+1} - \theta_{i,j}}{\Delta t} \qquad \textbf{19.}$$

When implementing this into the diffusion equation, there are two options. Taking the second derivative in time j or in time $j + 1$.Both ask for a different solving method, respectively the explicit method and the implicit method. Both methods are displayed in a stencil in figure 10.

This method can be explained with the use of a stencil representing the two. The deflections at time j are known, the deflections at $j + 1$ are asked.

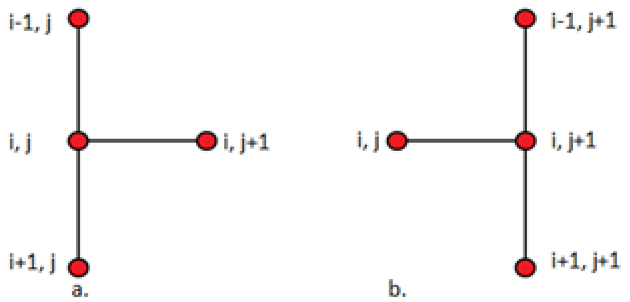

FIGURE 10: STENCIL REPRESENTING A) THE EXPLICIT METHOD AND B) THE IMPLICIT METHOD

Both methods are equally capable in solving the regular diffusion equation. Both will be elaborated on in the following paragraphs.

3.1.1 The explicit method

The explicit method calculates with the use of three different points, one point in the next time step. Mathematically it looks like this.

$$\theta_{i,j+1} = \frac{D \cdot \Delta t}{\Delta s^2}\left(\theta_{i+1,j} - 2\theta_{i,j} + \theta_{i-1,j}\right) + \theta_{i,j} \qquad \textbf{21.}$$

The first term of this expression is also known as the Fourier number. This number is crucial for solving the equation.

$$F = \frac{D \cdot \Delta t}{\Delta s^2} \leq 0.5 \qquad \textbf{22.}$$

For having a stable reliable solution, the Fourier number should be lower or equal to 0.5. Translated to the physical relation this means that the beam will bend the right way. When the Fourier number exceeds 0.5, the specimen will bend according to the red line in figure 11.This shape does not makes sense in physical context and it will result in an unstable result.

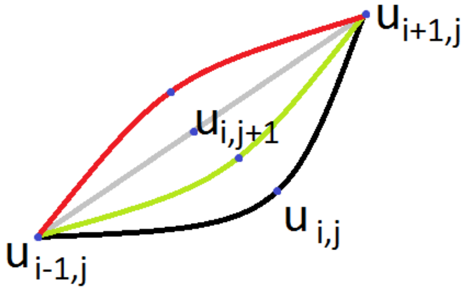

FIGURE 11: PHYSICAL EXPLANATION OF THE FOURIER NUMBER

The Fourier number is dependent on the size of the time step, space step and of the diffusion coefficient. In regular cases this condition is within reach, which makes it a favorable approach, because it is numerically stable and also less intensive for large calculations [13]. In most cases this is a good choice for the calculations. However in this case, the Fourier number becomes too complicated to find a suitable space and time step size.

3.1.2 The implicit method

The implicit method is a more numerical intensive solving method. Instead of a direct equation for a next point, this method is based on matrix calculations. These matrix calculations are based on the mathematical principle that a set of equations can be solved, if the amount of equations is equal to the amount of unknowns.
In this method the equation will be separated in a matrix with variables and two vectors, one containing the unknown angles of the current time step, one containing the boundary conditions and information about the previous time step.

$$-\frac{D \cdot \Delta t}{\Delta s^2}\,\theta_{i+1,j+1} + \left(\frac{2 \cdot D \cdot \Delta t}{\Delta s^2} + 1\right) \cdot \theta_{i,j+1} - \frac{D \cdot \Delta t}{\Delta s^2}\,\theta_{i-1,j+1} = \theta_{i,j} \qquad \textbf{23.}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -F & 1+2\cdot F & -F & 0 & 0 & 0 \\ 0 & -F & 1+2\cdot F & -F & 0 & 0 \\ 0 & 0 & -F & 1+2\cdot F & -F & 0 \\ 0 & 0 & 0 & -F & 1+2\cdot F & -F \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} \theta_{1,j} \\ \theta_{2,j} \\ \vdots \\ \vdots \\ \theta_{N-1,j} \\ \theta_{N,j} \end{bmatrix} = \begin{bmatrix} 0 \\ \theta_{2,j-1} \\ \vdots \\ \vdots \\ \theta_{N-1,j-1} \\ \frac{\omega}{2} * j * \Delta t \end{bmatrix} \qquad \textbf{24.}$$

The matrix and the vector on the right hand side are known, therefore the local deflection angles can be calculated. This method has been proved, suitable for a variable diffusion coefficient.

3.2 Defining parameters with a variable viscosity

The diffusion coefficient is defined as a function of the viscosity. As seen in the previous chapter the viscosity is not constant, but a function of the shear rate (equation 17).
Looking into the literature, this relation describes the power-law of fluid, also known as the Ostwald-de-Waele relationship.

$$\tau = K\,\dot{\gamma}^{n} = \eta\,\dot{\gamma} \Rightarrow \eta = K\,\dot{\gamma}^{n-1} \Rightarrow m = n - 1 \qquad \textbf{25.}$$

The relation between the shear rate and the rate of the deflection angle, is described in equation 1.

When these relations are substituted in the diffusion coefficient, the diffusion coefficient has become a function of the rate of deflection angle.

$$D = \frac{EI_f}{W\left(h_f + h_m\right)\left(1 + \frac{h_f}{h_m}\right)^{1+m} K\dot{\theta}^{m}} \qquad \textbf{26.}$$

3.3 Solving method

Due to the shear rate dependency of the diffusion coefficient, its value becomes also unknown and has to be solved for each position in each time step. In order to find the diffusion coefficient for each time step an iterative scheme is applied, shown in figure 12.

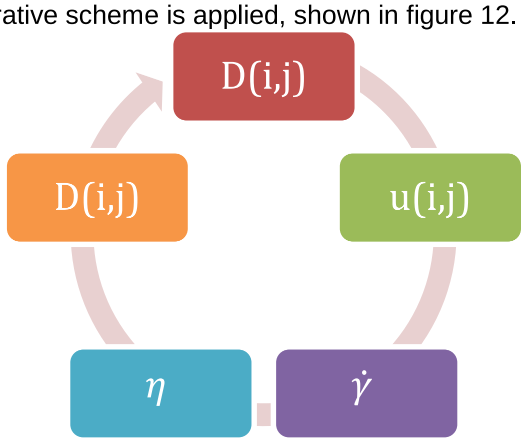

FIGURE 12: ITERATION SCHEME

With the use of a guessed diffusion coefficient the matrix (equation 24) is filled. The right hand side is filled with the first boundary conditions at $j = 0$. Using the inverse matrix equation the new deflection angles are calculated. With the deflections at the previous time step the angular velocity of deflection is calculated for each space step, as well as the shear rate, the viscosity and the new diffusion coefficients. These coefficients are compared to the guessed ones and the error between the two is calculated. When the error is too large the calculations are done again, instead of guessing, this time the new diffusion coefficients will be placed in the matrix. The deflection angles are recalculated and the process as shown in figure 12, starts again. This cycle will be repeated until the largest error of the space steps is small enough. When this is achieved, a new time step will be calculated. The boundary conditions at the right hand side are replaced by the angles of the previous time step.

In order to prevent the loop continuing on infinitely, the error is set at $1 \cdot 10^{-10} \frac{m^2}{s}$, approximately $0{,}01\%$ of the first guessed diffusion coefficient.

A problem with this method occurs when there is no shear. This makes the matrix in equation 24 singular and therefore it cannot be solved. To prevent this a minimum of $1 \cdot 10^{-15}$ is applied. Every diffusion coefficient below this minimum will be defined at this minimum. Apart from this minimum there is also a maximum amount of iterations given. This prevents the script from getting stuck in a loop.

3.4 Validation of the numerical model

To check if the results are valid three different actions are taken.
First the result will be checked for the situation where the diffusion coefficient is known. The diffusion coefficient must be zero around $s = 0$ for the first time steps. The diffusion coefficient also ends at a prescribed value, as the angular velocity of the shaft is known. When this is correct, it can be stated that the matlab script does not contain errors with the boundary conditions.

The second validation step is by increasing the number of time steps and space steps. According to the finite difference method, when the amount of steps becomes infinite the results will be exact. Thus by increasing the steps the results become more accurate. However the basic shape should not differ that much between 200 and infinity. When this is correct, it can be stated that the solution is converging if the discretization steps are made smaller.

The last step will consist of increasing the iteration steps. According to the iteration method, if infinitely many steps are made the right answer will be found in theory, but it can also become stuck in a loop. To validate the results the amount of iterations can be increased, this could not affect the basic shape of the result. With this method a suitable amount of iterations can be chosen to run the script on.

4 RESULTS

4.1 The local deflection angle

With the numerical analysis a prediction is made for the shape of the specimen and the deflection angle at multiple time steps during the bending process (figure 13). This prediction is for a specimen with a fiber layer with a Young's modulus E of 230 GPa, a second moment of area I_f of 7.1458·10^{-19} m^4, both the fiber and matrix layer have a height of 7µm (h_f, h_m), the length L is 15 mm and the width W is 25 mm. For the relations in the power-law of fluid, the flow behavior index n is 0.3391 and the flow consistency index K is 9.3663kPa·s^n

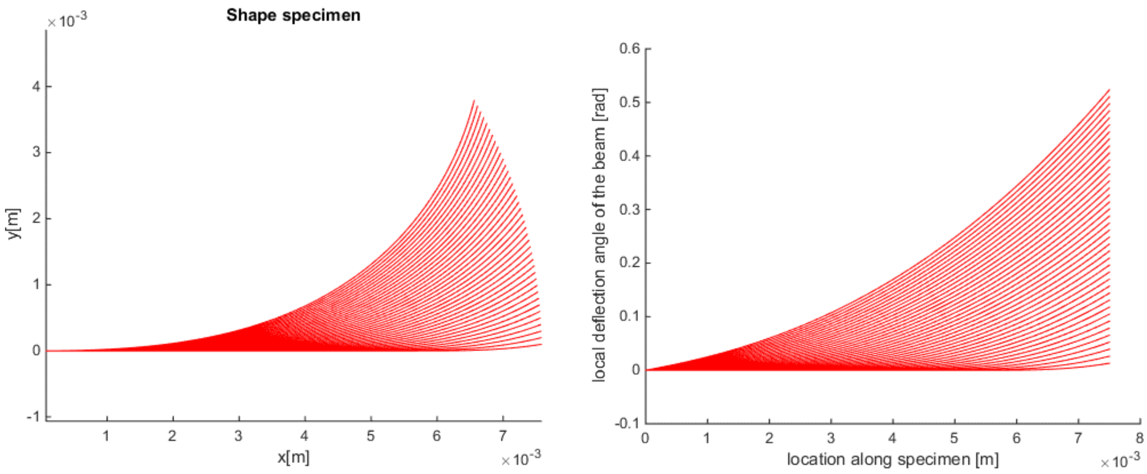

FIGURE 13: THE SHAPE OF THE SPECIMEN (A) AND ITS DEFLECTION ANLGE (B) AT DIFFERENT TIME STEPS

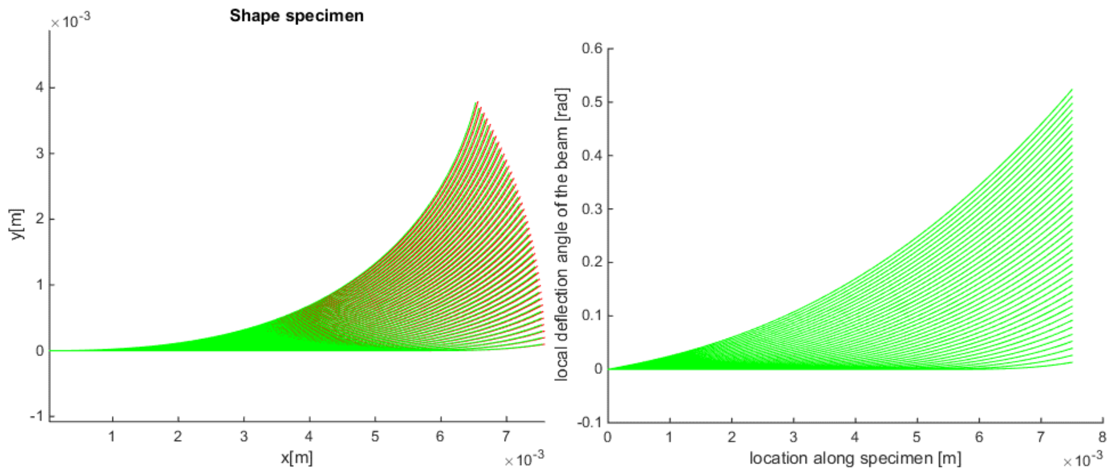

FIGURE 14: THE SHAPE OF THE SPECIMEN (A) AND ITS DEFLECTION ANGLE (B) AT DIFFERENT TIME STEPS. RED N = 100, GREEN N = 200

In figure 14 these results of figure 13 are compared to the results with a finer grid In the local deflection angle, it can be stated that the difference is very small, as there is no red visible to the eye. When zoomed in a small difference can be detected as seen in figure 15.

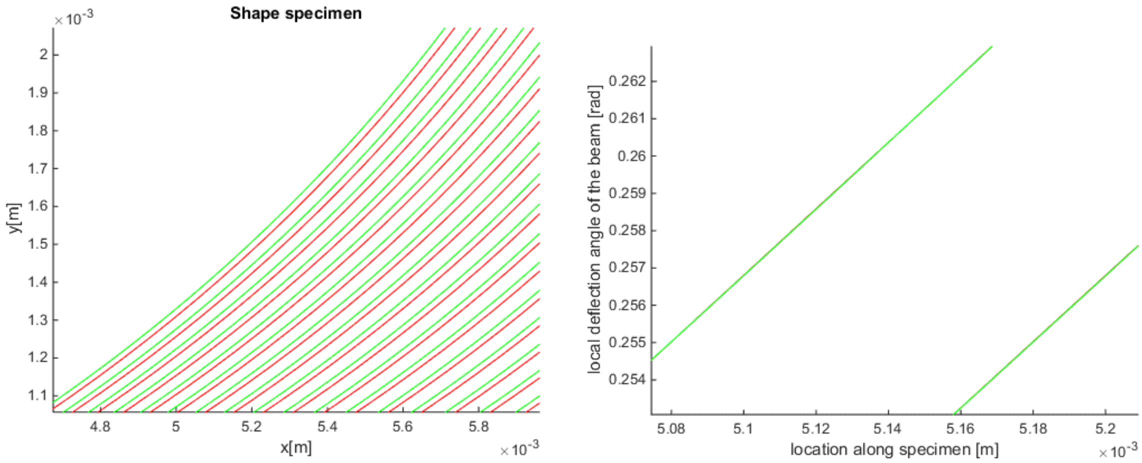

FIGURE 15: A ZOOM IN FIGURE 14

When looking at the shape of the plot with the deflection angle (figure 13b), it is clear that the specimen will not bend with a linear deflection angle. Comparing the results of a linear deflection with the results found, it is found that the actual shape is a bit more sagged, see figure 16.

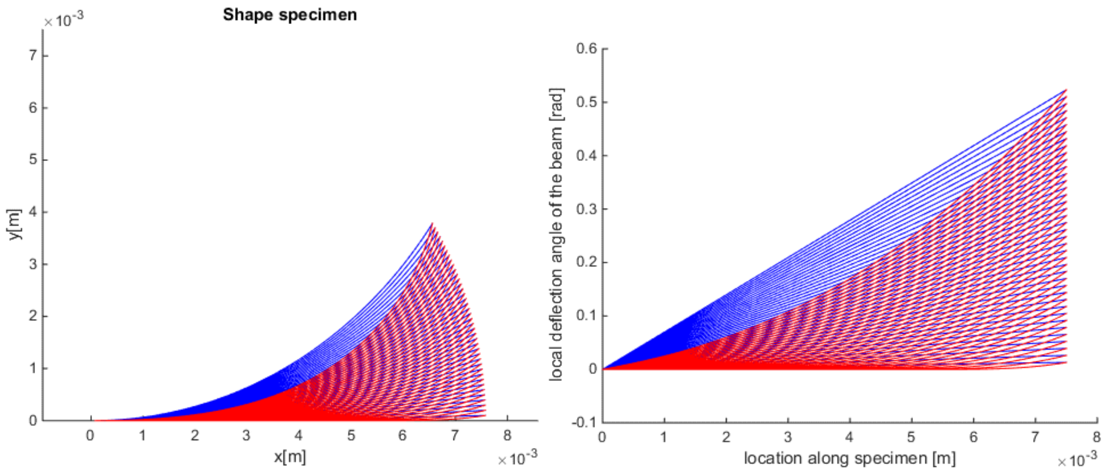

FIGURE 16: THE RESULTS COMPARED TO LINEAR BEHAVIOR

Note that the results during the bending process are presented. It is clear that the specimen does not have its final shape at the end of the bending process.
At time $t = \infty$, the specimen will have a complete linear bend. In this case, because the bending will take place in seconds, the bend is as good as linear after 5 minutes, see figure 17.

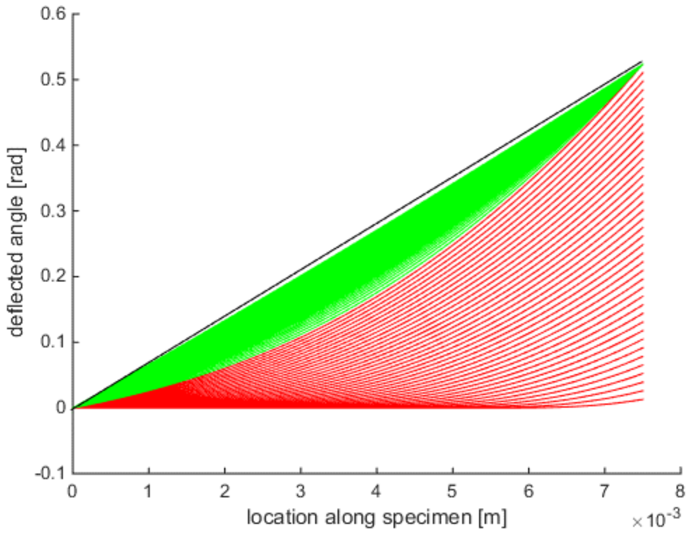

FIGURE 17: DEFLECTION OF THE SPECIMEN, RED SHAPES DURING BENDING PROCESS ENDING AT 1 SECOND, GREEN SHAPES AFTER BENDING PROCESS ENDING AT 26 SECONDS, THE BLACK LINE REPRESENTS A PERFECT BEND.

4.2 Diffusion coefficient

The behavior of the specimen can be explained by looking at the diffusion coefficient. Recalling that a diffusion coefficient approaching zero is very reluctant to bending and that a higher diffusion coefficient represents a less reluctant bending. The plot of the diffusion coefficient (figure 18) can explain a lot about the behavior inside the specimen, as it is related to the shear stress.
The diffusion coefficient increased along the specimen and in time.

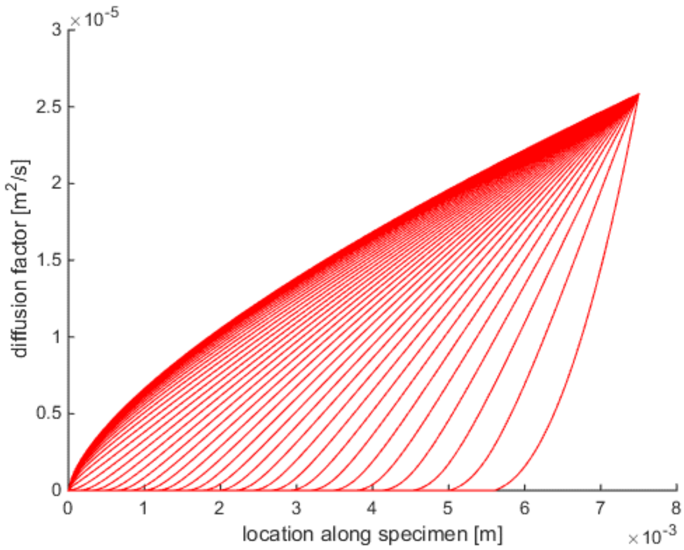

FIGURE 18: THE DIFFUSION COEFFICIENT LONG THE SPECIMEN AT DIFFERENT TIME STEPS.

At the first few steps the diffusion coefficient is in the early time steps approximately zero. This is because at these locations, the deflection has not reached yet. As described in equation 29, the diffusion coefficient is related to the local rate of deflection at space step i and time step j. So when $\dot{\theta}$ is zero, the diffusion coefficient is zero as well.

When time continues, the diffusion angle will become constant for an individual location i. Every point begins and ends at the same diffusion coefficient. At $s = 0$, the beam is fixed, results in a diffusion coefficient of 0. At $s = \mathrm{L}$ the diffusion coefficient is constant. This is because $s = \mathrm{L}$ is the last point inside the clamp which moves at a constant speed. The shear rate is always the same and thus also the diffusion coefficient.

Looking at the points in between, it is clear that the local rate of deflection keeps increasing when time continues; first at a higher pace and then increasing more slowly, but the rate keeps increasing.

After the bending shaft has stopped, there is a large change in the diffusion coefficient. The tip at $s = \mathrm{L}$ drops to zero the moment the shaft stops, because the rate has become 0. This also causes that the diffusion coefficient drops starting at point $s = 0{,}7\ \mathrm{L}$, when approaching infinity the peak starts going to $s = 0{,}5\ \mathrm{L}$, slowly becoming a straight zero line.

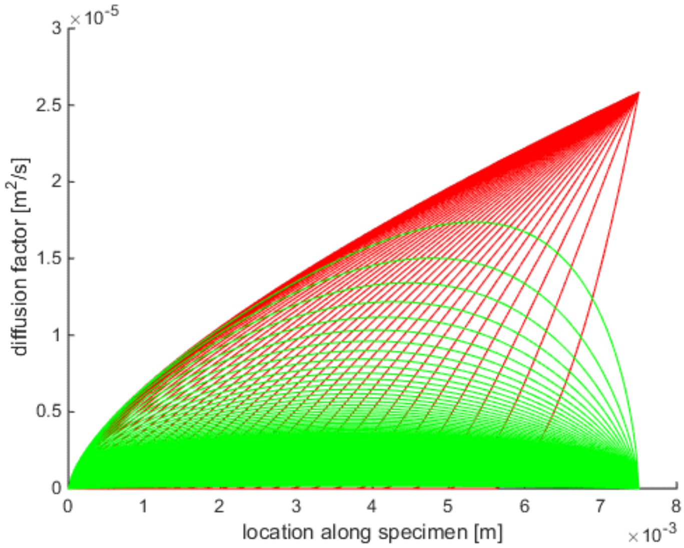

FIGURE 19: DIFFUSION COEFFICIENT ALONG THE SPECIMEN AT DIFFERENT TIME STEPS. RED: DURING BENDING TO 1 SECOND, GREEN: POST BENDING TILL 1.5 SECONDS

4.3 Shear stress and force

When translating the diffusion coefficient to the shear stress, it is proven that when the diffusion coefficient increases, the shear stress increases as well. Due to their relation increasing rate of the shear stress is will increase according to equation as in equation 25.

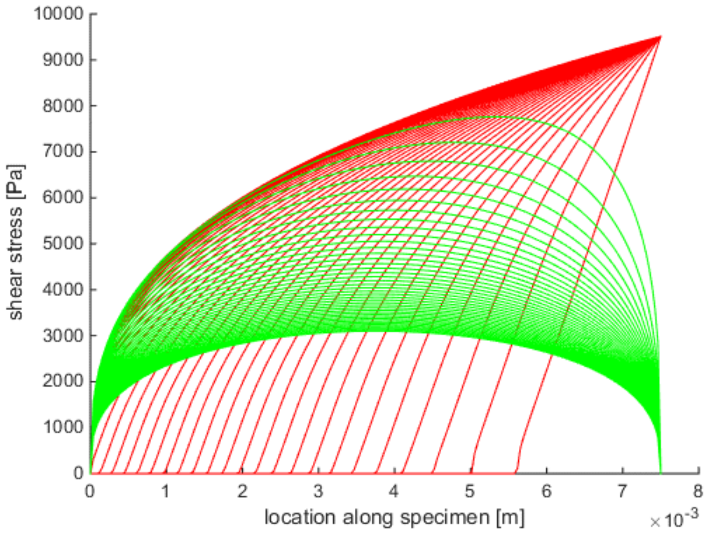

FIGURE 20: SHEAR STRESS ALONG THE SPECIMEN AT DIFFERENT TIME STEPS AND AFTER BENDING PROCESS

The sudden drop in shear stress at $s \to L$ has no large consequences for the last deformation of the specimen. This part of the beam is already very close to its final deflection.

5 DISCUSSION

5.1 Comparison to the old model

With this new model there is a more accurate model for the deformation of a thermoplastic composite during the bending process. When comparing this model to the previous simplified model of Sachs, there are noticeable differences.
First of all, the value of the viscosity was a guess in the old model, with the new model the diffusion factor and with it the viscosity is defined. The results give an accurate result of the whole specimen, as it is only dependent on measurable constants.

When looking at the deflections of the new model compared to the old model (figure 21), it is clear that when $s \to L$, the old and the new model start to deflect more alike. This can be explained by looking at the diffusion coefficient (figure 18). The diffusion coefficient increases to a constant value.
At $s \to 0$, deflection differs. The old model predicted that the beam would deflect at a higher rate, when $s \to 0$, however the new model corrects this. Due to the shear-thinning viscosity, the onset of the deformation is hindered. And the deflection becomes more concentrated at the clamped side of the specimen, where the deformation started.

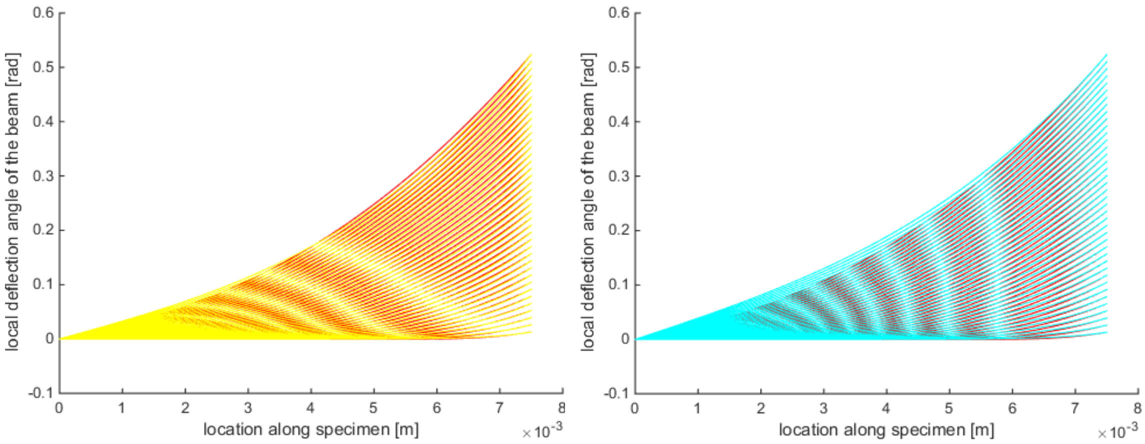

FIGURE 21: THE DEFLECTION ANGLE FOR IN RED THE NEW MODEL, THE OLD MODEL IN YELLOW WITH D=1.6E-5 AND IN CYAN WITH D= 2E-5

5.2 Comparison to experimental results

The direct results of this new model cannot be instantly checked with experimental results. Local deflection angles are hard and often inaccurate to measure. Measuring the shear stress for every component is impossible.
To check the data with experimental values, the moment caused by the bending must be calculated, as this is a value that can be measured by the rheometer.

As can be seen in figure 9 the moment starts at 0, then steeply climbs up to a constant rate, which starts increasing at the end of the bending process. In order to validate the results completely the moment must be calculated. The equation Sachs used for his prediction is not suitable for the new equation, since the equation has become non-linear. The next step predicting the behavior of thermoplastic composites when being bended, should be to determine the moment exerted on the shaft according to this new model.

5.3 The effect of thickness and temperature

When taking a closer look at the new equation, the model is not a direct function of temperature and of the thickness of the specimen. Looking at the results of experiments, these two factors do play a role when translating to the moment exerted on the shaft.
Combining these two statements and the assumption made that the height is significantly small in comparison to the bending radius, it can be concluded that the thickness only plays a role in the equation from local deflection angle towards the exerted moment. This corresponds with the method of Sachs.

The temperature does bring along some problems. In the model of Sachs the temperature also was not taken into account in either the diffusion equation or in the calculation of the exerted moment. However the viscosity chosen by him could very well differ at times. When researching viscosity, a clear relation between the viscosity and temperature was found especially considering melts [7]. This would state that the temperature should play a role in the deformation angle. As it is known that the viscosity is probably influenced by the temperature the calculation of the viscosity has a function of temperature.
In this research, the data to determine the exact relation between the viscosity and the shear rate, came from the research Sachs has done with Victrex PEEK 150P thermoplastic layer bent at a temperature of 385 °C. Looking at figure 10, there are slightly different relations measured for other thermoplastic layers at different temperatures.
To conclude, the temperature has an influence on the flow consistency index and the flow behavior index. Both these indexes are used to determine the relation between the shear rate and viscosity. At different temperatures and with different thermoplastics different values have to be used.

5.4 Assumption check

To set up the diffusion equation assumptions where made, to check the validity of the results these assumptions have to be checked to see if they fit the results.

"The thickness of the laminate H is small in comparison to the bending radius ρ: $\frac{H}{\rho} \ll 1$."
This assumption is still true, the thickness and bending radius have not changed.

"This implies that: $ds \approx ds_i$, where i is the layer index."
As can be seen in de shape of the specimen and in the model (figure 4 and 13), the laminate will be pulled out of the fixture. This was also the case in the simplified model. This deformation is however small enough to assume that the little differences in step size, will not have any large repercussions.

"The matrix layer can only carry shear forces."
This assumption is still true, the viscosity of the matrix layer is likewise affected by the shear forces.

"The fiber layer deform due to bending moments."
This assumption is still true.

"The matrix is a Newtonian viscous fluid with viscosity η."
This assumption is not true and is the base of the improvement of the model.

“The fiber is a Hookian elastic solid with elastic modulus E.”
This assumption is still true.

“The deformation of the laminate is considered small. Thus neglecting non-linearity by deformation.”
This assumption is still true, see assumption 2.

“All fiber layers deform equally: $M = M_i$ and $dM = dM_i, \forall i.$”
With these results this assumption is hard to validate. The results gained do not invalidate this result, however it does give insight in the complexity of the resistance within the laminate to bend. This could affect the moments in the different layers. This assumption is neither validated nor invalidated.

“All matrix layers deform equally: $Q = Q_i$ and $dQ = dQ_i, \forall i.$”
With these results this assumption is hard to validate. The results gained do not invalidate this result, however it does give insight in the complexity of the resistance within the laminate to bend. This could affect the moments in the different layers. This assumption is neither validated nor invalidated.

6 CONCLUSION AND RECOMMENDATIONS

With the use of the elaborated diffusion equation a more accurate model is made to predict the behavior during the production process. When the moment exerted on the shaft is modeled with the new results, a more accurate bending process can be designed. With this moment it can be seen how much the resistance is to bend, this resistance might have a relation with formability problems, like wrinkling.

Researching the influence of the temperature on the viscous behavior of the matrix layer, gives an extra dimension to the solution. Apart from knowing how the results differ at different temperatures, it might also give an inside on how temperature regulation can help prevent buckling and better the bending results.

In this report the influence of the speed of the rheometer was not discussed. This has interesting results for the behavior of the specimen as can been seen in figure 20 at different speeds in rotations per minute. When the angular velocity increases the resistance lowers. This behavior can be used in developing an ideal production process.

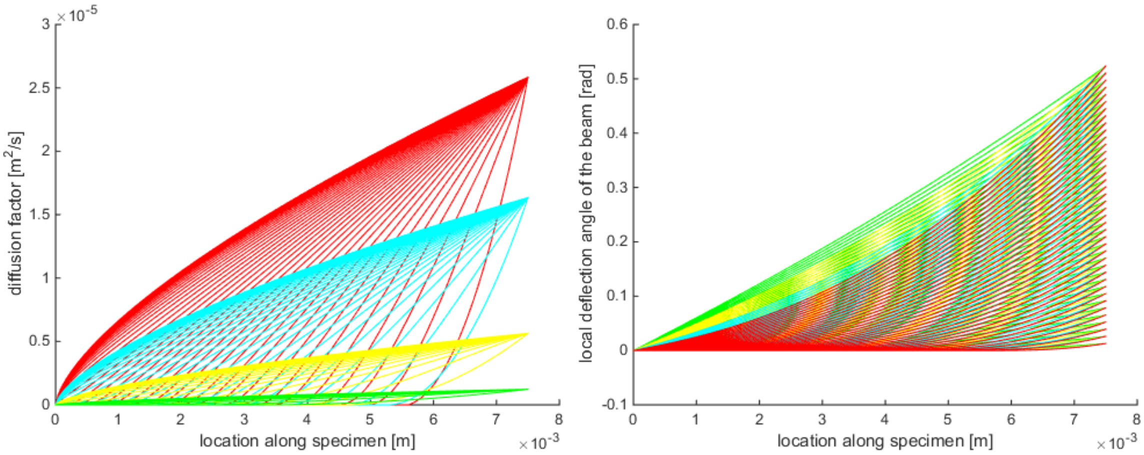

FIGURE 22: THE DIFFUSION COEFFICIENT AND DEFLECTED ANGLES AT GREEN: 0.1 RPM, YELLOW: 1 RPM, CYAN: 5 RPM, RED: 10 RPM

All together a more accurate model is built to predict the behavior of thermoplastic composites. This new model has given more insight in the shear forces playing within the layers in the laminate. It is also a base on which the exerted moment can be calculated, which will give more insight in how to handle the bending process of thermoplastic composites.

7 APPENDIX

7.1 Summation of variables

α	Angle of bending shaft	(rad)
γ	Shear	-
$\dot{\gamma}$	Shear rate	(1/s)
η	Viscosity	(Pa·s)
θ	Local deflection angle	(rad)
$\dot{\theta}$	Rate of angle deflection	(rad/s)
τ	Shear stress	(Pa)
ω	Angular velocity of the bending shaft	(rad/s)
D	Diffusion coefficient	(m^2/s)
ds or Δs	Size of space step	(m)
dt or Δt	Size of time step	(s)
E	Young's modulus	(Pa)
F	Fourier number	-
h_f	Height of fiber layer	(m)
h_m	Height of matrix layer	(m)
I_f	Second moment of area in a fiber layer	(m^4)
i	Index of space step	-
j	Index of time step	-
K	Flow consistency index	(Pa·s^n)
L	Length of the specimen	(m)
m	*n*-1	-
M	Moment on the layers	(N·m)
M_c	Moment exerted on the shaft	(N·m)
n	Number of layers in the specimen	-
n	Flow behavior index	-
N	Normal force	(N)
N	Number of time steps	-
s	Location along the beam length	(m)
t	Time	(s)
V	Transverse force	(N)
W	Specimen width	(m)
Q	Shear force	(N)

7.2 Matlab script

```
%Solving parabolic equation of bending problem:
clear all
clc

%---- definition problem ----
%du/dt - D(du/dt) * d2u/dx2 = 0
%u = theta
%x = s

%---- define variables ----

Nx = 100; % number of points
Nt = 40; % [s] time step size
theta0 = 0; % [deg] left b.c.
alpha_end = 60/180*pi; % [rad] right b.c.
omega = 10*2*pi/60; % [rad/s] rotational velocity 0.1,1,5,10

k = 9.366314266817626e+03; % [Pa^-m*s^(-m-1)] flow consistency index
m = -0.660908018344660; % flow behavior index-1

%laminate dimensions
W = 25e-3; % [m] width specimen
H = 1e-3; % [m] hight specimen
L = 15e-3; % [m] length specimen

%material properties
v_f = 0.5; % fiber volume fraction
h_f = 7e-6; % [m] hight fiber layer
h_m =  h_f/v_f * (1-v_f); % [m] hight matrix
E = 230e9; % [Pa] Young's modulus
I = 1/12*W*h_f^3; % [m^4] Second moment of area
eta = 3.0137e+05; % [Pa.s] Viscosity
Dconst = E*I / (eta*(1+h_f/h_m)*(h_f+h_m)*W ); % [m^2/s] Diffusion
factor
C = Dconst*eta; % [Pa.m^2] Diffusion factor * Viscosity

%solving properties
Dmin = 1e-15; % [m^2/s] The minimal diffusion constant

t_end = alpha_end/omega; % [s] Duration bending process
dt = t_end/Nt; % number of time steps
t_space = 0:dt:t_end;

x_space = linspace(0,L/2,Nx);
dx = x_space(2)-x_space(1); % [m] space step size

Fo = Dconst * dt/ dx^2; % Fourier number

if Fo>0.5
    Fo;
end

%creating matrix
```

```
M = zeros(Nx,Nx);
RHS = zeros(1,Nx);
M(1,1) = 1; % left b.c.

eta = ones(Nx,1)*eta;
Fo = ones(Nx,1)*Fo;

for i = 2:Nx-1
    M(i,i-1:i+1)=Fo(i) * [-1 2+1/Fo(i) -1];
end
M(Nx,Nx) = 1; % right b.c.

u = zeros(Nx,1);
D = Dconst;

for j = 1:Nt
    fprintf(['time step ' num2str(j) '\n']);
    u_old = u;

    for iter = 1:40

        %update right hand side
        RHS = u_old;
        RHS(1) = 0;% left b.c.
        RHS(Nx) = omega/2*j*dt;% right b.c.

        solve u
        u = M\RHS;

        dudt = (u - u_old)./dt;
        D_old = D;

        D = E*I ./ (k * (1+h_f/h_m)^(m+1) * dudt.^m *(h_f+h_m)*W ) ;
        D(D<Dmin) = Dmin;

        error = max(abs(D_old-D));
        fprintf(['error ' num2str(error) '\n']);

        if error < 1e-10
            break
        end

        Fo = D * dt/ dx^2; % Fourier number
        for i = 2:Nx-1
            M(i,i-1:i+1)=Fo(i) * [-1 2+1/Fo(i) -1];
        end
    end


    for i = 1:Nx
        defly(i) = dx*i*sin(u(i));
        deflx(i) = dx*i*cos(u(i));
    end
```

```
    eta = D.\C
    tau = k.*(eta./k).^((m+1)/m);
    deriv_tau = diff(tau)./transpose(diff(x_space));
    deriv_D = diff(D)./transpose(diff(x_space));
    xd = x_space(2:length(x_space));
end

for j = Nt+1:Nt+40
    fprintf(['time step ' num2str(j) '\n']);
    u_old = u;

    for iter = 1:40

        update right hand side
        RHS = u_old;
        RHS(1)  = 0;% left b.c.
        RHS(Nx)  = omega/2*Nt*dt;% right b.c.

        %solve u
        u = M\RHS;

        figure(1)
        hold on

        dudt = (u - u_old)./dt;
        D_old = D;

        D = E*I ./ (k * (1+h_f/h_m)^(m+1) * dudt.^m *(h_f+h_m)*W );
        D(D<Dmin) = Dmin;

        error = max(abs(D_old-D));
        fprintf(['error ' num2str(error) '\n']);
        if error < 1e-10
            break
        end

        Fo = D * dt/ dx^2; % Fourier number
        for i = 2:Nx-1
            M(i,i-1:i+1)=Fo(i) * [-1 2+1/Fo(i) -1];
        end
    end

    eta = D.\C;
    tau = k.*(eta./k).^((m+1)/m);
    deriv_tau = diff(tau)./transpose(diff(x_space));
    deriv_D = diff(D)./transpose(diff(x_space));
    xd = x_space(2:length(x_space));

    for i = 1:Nx
        defly(i) = dx*i*sin(u(i)); %coordinate y for the shape
        deflx(i) = dx*i*cos(u(i)); %coordinate x for the shape
    end

end
```

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