A Representative Volume Element Simulation Of A Thermo Plastic Elastomer

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Appendix A 1
Abstract

Thermoplastic elastomers (TPE) are a class of copolymers or a physical mix of polymers, usually a plastic and a rubber, which consist of materials with thermoplastic and elastomeric properties. The advantage of a TPE is the combination of easy processing, just like engineering thermoplastics, with excellent mechanical properties and the flexibility of rubbers. A main application area is the automotive industry; TPE is for example used in bushings, airbag covers, brake tubes, air ducts and cables.

In order to describe the strain-stress behavior of a TPE, the material is modeled as a Representative Volume Element (RVE). This element describes the homogenous behavior of the two phases, the rubber and the thermoplast, inside the RVE. For the thermoplastic phase the so called Eindhoven Glassy Polymer (EGP) model is used, which has been updated in 2007 to a multi-mode approach for improved accuracy in the pre-yield regime.

The RVE is modeled in 2D in the finite element package MSC MARC/Mentat. Simulations are carried out with a variety of parameters, such as material parameters, inclusion size and inclusion percentage in order to predict the parameters of an experimentally tested TPE. In a later stadium the results are compared with the software package DIGIMAT, this is homogenization software for linear and nonlinear multi-scale material modeling. The simulations are partially done in a combination with the finite element package ABAQUS/CAE.
Notation

\( \alpha, a, A \) scalar
\( A \) second order tensor
\( I \) second order unity tensor

Operations

\( A^c \) conjugate or transposed
\( A^{-1} \) inverse
\( \text{tr}(A) \) trace
\( \text{det}(A) \) determinant
\( A^d = A - \frac{1}{3} \text{tr}(A)I \) deviatoric part
\( A^h \) hydrostatic part
\( \tilde{A} \) isochoric part
\( \dot{A} \) material time derivative
\( AB \) dyadic product
\( A \cdot B \) inner product
\( A : B = \text{tr}(A \cdot B) \) double inner product
\( \delta \) variation
\( \partial \) partial derivative
Chapter 1

Introduction

Thermoplastic elastomers (TPE) are polymeric materials that consist of a combination of a thermoplastic material and an elastomeric rubber. This gives also a combination of their properties. The material is processable like typical thermoplastics; this means that processes like injection molding, extrusion and blow molding are possible. Recycling of the product and the scrap, which is produced during production, is also possible, in contrary to the processing of rubbers. (See Figure 1.1) The mechanical properties are comparable to rubbers with its typical flexibility and elasticity.

Figure 1.1 The processing of rubbers vs. TPE's.

TPE’s can be made out of two concepts. The first one is combining an elastomer and a thermoplastic in a polymerchain by using block copolymers. With this method the result is a one-phase TPE. (See Figure 1.2) Another concept is compounding. The rubber and thermoplastic material are mixed in a blend with a two-phase TPE as result.
In these methods are many variations possible, such as the volume percentage of the elastomer and the type of the thermoplast and the elastomer. With these variations a TPE material can be developed which is best suited for a certain application. At this moment the main application area is the automotive industry. DSM developed a polyester based TPE, called Arnitel. This material is already applied in a number of products such as in an airbag cover, brake tubing, air ducts, seals and cabling. (See Figure 1.3) TPE’s can also be applied in non-automotive products, such as a wine press tapes and railway pads. (See Figure 1.4)

Arnitel has the following properties:
- Excellent fatigue endurance
- High peak temperature resistance
- High impact strength
- Good resistance to chemicals and weathering
- High tear and abrasion resistance
- Good tactile feel
- High load bearing capacity
- Excellent overmoulding adhesion (abs/pbt/pc/metals)

Figure 1.2 AFM images of a one-phase TPE (left) and a two-phase TPE (right)

Figure 1.3 Examples of Arnitel applications in the automotive industry; airbag cover, air ducts and seals.
Figure 1.4 Non-automotive applications of Arnitel; wine press taper, tools, railway pads.
Chapter 2

The representative volume element

The TPE, as mentioned previously can be modeled with a so called Representative Volume Element (RVE). In this chapter the main principles of an RVE model will be explained.

2.1 Homogenization

Consider a heterogeneous body of the TPE material. That body consists of a blend of two materials, a stiff glassy polymer such as polycarbonate (PC) with soft rubber inclusions. When an external load is applied to the body, the real deformation and stress fields show large gradients and discontinuities because of the inclusions. Assuming that these inclusions are very small compared to the body dimension, the deformation field in the vicinity of one inclusion will be approximately the same as the deformation field near neighboring inclusions. This suggests that the macroscopic stress-strain relation at a certain point P can be determined by applying the local macroscopic stress-strain relations to a micro structural spatially RVE at to P in such a way that the RVE strains are equal to the local macroscopic strains and by averaging the non-uniform RVE stress field. This implies that a new homogeneous material is created with approximately the same mechanical behavior as the original heterogeneous material. [1]
2.2 Numeric modeling

The generation of the RVE is done using the finite element software package MSC Marc/Mentat. For the simplicity an RVE is chosen of 1x1x1 mm. The RVE is composed of a polymer matrix containing different volume fractions of (soft) rubber inclusions. In the simulations volume fractions are used from 50% up to 70%. The EGP-model, as proposed by Den Hartog [2] that is used to describe the matrix material is only available for plane strain conditions, so the RVE is a 2D model with plane strain boundary conditions. The RVE model that is used in most cases of the simulations can be seen in Figure 2.1, with the middle sphere situated off-centre. One RVE consist of about 800 8-noded plane strain quadrilateral elements. This is element type number 27 in MSC Marc. The use of these elements proved to be necessary in order to give accurate results because of the combination of the used material model together with excessive deformations inside the RVE structure [3].

To prevent rigid body movement during simulations, the lower left node is fixed in x- and y-direction, whereas the top left node is fixed in y-direction.

In order to regard the RVE as a representative part of a whole structure, it is assumed that representative cell deforms in a repetitive way identical to its neighbors. For a 2-D RVE this implies that the shape of both boundaries, bottom-top and left-right, is and remains identical to each other and that the stresses acting on these boundaries are equal, but opposite in sign. In Marc/Mentat this can be done with so-called Servo Links. According to Smit [1] this method can be summarized as follows:

- The shape of both boundaries (bottom-top and left-right) must remain identical. This can be done by tying the nodes on the left boundary $\Gamma_{14}$ (See Fig. 2.1) to their corresponding notes on the right boundary $\Gamma_{23}$ and to the corner notes 1 and 2. Also the notes on the upper boundary $\Gamma_{43}$ have to be tied to the notes on the lower boundary $\Gamma_{12}$ and to the corner notes 1 and 4. In formula;

  \[
  y_{\Gamma_{14}} = y_{\Gamma_{23}} - y_2 + y_1 \\
  y_{\Gamma_{43}} = y_{\Gamma_{12}} - y_4 + y_1
  \]  

  with $y_{\Gamma_{ij}}$ as the position vector of point on edge $\Gamma_{ij}$.

- As mentioned before, the stress vectors on two opposite boundaries are equal but opposite in sign. With $\sigma \cdot n$ as the stress vector acting on a boundary with outward normal n, this condition can be modeled as

  \[
  \sigma \cdot n_{\Gamma_{14}} = -\sigma \cdot n_{\Gamma_{23}} \quad (2.3) \\
  \sigma \cdot n_{\Gamma_{12}} = -\sigma \cdot n_{\Gamma_{43}} \quad (2.4)
  \]
In order to deform the RVE, only the lower right node of the RVE is given a prescribed displacement. This is because of the applied periodic boundary conditions. All the loadings are at a strainrate of $10^{-2}$/s. At a certain specified strain, the node is released and unloads until a zero stress level is reached. This can be done by implementing the option “release node” in the loadcase.

As output, MSC Marc gives the displacement and the resulting force of the RVE. Because of the unit dimensions, this output can be directly translated to engineering strains and stresses according to:

$$\sigma_{\text{eng.}} = \frac{F}{A_0} = \frac{F}{1} = F$$  \hspace{1cm} (2.1)

$$\varepsilon_{\text{eng.}} = \frac{\Delta l}{l_0} = \frac{\Delta l}{1} = \Delta l$$  \hspace{1cm} (2.2)
Chapter 3

Material models

The RVE that is used in the simulations consists of two different materials. The matrix is modeled by the EGP material presents a thermoplastic polymer while the elastomeric inclusions are described by a neo-Hookean model. In this section the specific used material models will be explained.

3.1 The matrix material

As mentioned above the matrix consists of a thermoplastic polymer. The constitutive model for these kind of amorphous polymers is based on the derivations of Den Hartog[2], who modified the model introduced by Klompen[4] by extending it to a multi mode model. The equations are derived for a thermo-rheological simple material and for an arbitrary number of nodes, n. This number is unknown on beforehand and will vary for different materials.

In Figure 3.1 one can see a graphically representation of a single and multi mode model by using spring/dashpot combinations.

![Figure 3.1 Schematic representation of the single (left) and multimode (right) model build up of springs and dashpots](image)
3.1.1 Kinematics

In order to derive the constitutive equation some kinematic properties and assumptions are needed. In the following these relations are presented and derived.

Based on Leonov [5] the deformation gradient tensor $F$ can be multiplicatively decomposed into an elastic part $F_e$ and a plastic part $F_p$:

$$ F = F_e \cdot F_p $$  \hspace{1cm} (3.1)

Because the rotational contributions are neglected, this decomposition is not unique. In order to guarantee uniqueness, an extra assumption is needed.

Assume that during plastic deformation, the volume change is zero, this implies:

$$ J_p = \det(F_p) = 1; \quad J = \det(F) = \det(F_e) $$  \hspace{1cm} (3.2)

The isochoric (volume-preserving) elastic deformation can now be written as:

$$ \tilde{F}_e = J^{-1/3}F_e $$  \hspace{1cm} (3.3)

As a strain measure the left Cauchy Green strain tensor $B$ is used, when combining this with the equations above, the isochoric elastic part of the left Cauchy Green tensor can be calculated:

$$ B = F \cdot F^c, \quad \tilde{B}_e = \tilde{F}_e \cdot \tilde{F}_e^c $$  \hspace{1cm} (3.4)

The velocity gradient $L$ can be additively split in two parts, the deformation rate tensor $D$, and a skew-symmetric part, the spin tensor $\Omega$. With the multiplicative decomposition of $F$, $L$ can also be split up into an elastic and plastic part.

$$ L = \dot{F} \cdot F^{-1} = D + \Omega $$  \hspace{1cm} (3.5)

$$ L = \dot{F}_e \cdot F^{-1}_p \cdot F^{-1}_p + \dot{F}_p \cdot F^{-1}_p \cdot F^{-1}_p = L_e + L_p $$  \hspace{1cm} (3.6)

$$ L_e = \dot{F}_e \cdot F^{-1}_e = D_e + \Omega_e $$  \hspace{1cm} (3.7)

$$ L_p = F_e \cdot \dot{F}_p \cdot F^{-1}_p \cdot F^{-1}_p = D_p + \Omega_p $$  \hspace{1cm} (3.8)
3.1.2 Stress calculation

Conservation of momentum, moment of momentum and mass, represented by the balance laws have to be satisfied both in space as in time.

\[
(\vec{V} \cdot \sigma) + \vec{q} = 0; \quad \sigma = \sigma^c \quad \text{and} \quad \rho J = \rho_0; \quad \text{in} \Omega, \forall \tau \leq t \quad (3.9)
\]

Where \( \sigma \) is the Cauchy stress, \( \vec{q} \) the body force per unit of volume, \( \rho \) the mass density (with \( \rho_0 \) as the initial mass density), \( J \) the volume change ratio and \( t \) denotes the current time. Without additional constitutive equations and boundary conditions this set cannot be solved.

The Cauchy stress tensor \( \sigma \) is additively divided into a driving stress tensor \( \sigma_s \) and a hardening stress tensor \( \sigma_r \).

\[
\sigma = \sigma_s + \sigma_r; \quad \text{with} \quad \sigma_s = \sigma_s^d + \sigma_s^h \quad (3.10)
\]

![True stress-strain curve](image.png)

**Figure 3.2a)** True stress-strain curve  \quad **b)** corresponding graphical representation

The total driving stress tensor, for the multi mode model, is the sum of the driving stress tensor for each mode individually, \( \sigma_{s_i} \). This tensor can be further divided into the modal deviatoric part \( \sigma_{s_i}^d \) and the modal hydrostatic part \( \sigma_{s_i}^h \) according to Equation 3.11. The subscript \( i \) stands for a specific mode, \( i = [1, 2, \ldots, n] \).
\[ \sigma_s = \sum_{i=1}^{n} (\sigma_{s_i}) = \sum_{i=1}^{n} (\sigma_{s_i}^d + \sigma_{s_i}^h) \]  
(3.11)

\[ \sigma_{s_i}^d = G_i \tilde{B}_{e_i}^d \]  
(3.12)

\[ \sigma_{s_i}^h = \kappa_i (J - 1) I \]  
(3.13)

Where in the deviatoric part \( G_i \) denotes the shear modulus and \( \tilde{B}_{e_i}^d \) the deviatoric part of the elastic isochoric left Cauchy Green strain tensor. In the hydrostatic part, \( \kappa_i \) is the bulk modulus, \( J \) the total volume change ratio and \( I \) the unity tensor.

The hardening stress is described with a Neo-Hookean relation, where \( G_r \) is the hardening modulus and \( \tilde{B}_r^d \) the deviatoric part of the isochoric left Cauchy Green deformation tensor.

\[ \sigma_r = G_i \tilde{B}^d \]  
(3.14)

Because of the time and history dependence of the model, it is necessary that the volumetric and elastic strain changes are calculated through the evolution equations for \( J \) and \( \tilde{B}_{e_i}^d \).

\[ \dot{J} = J \text{tr}(L) \]  
(3.15)

\[ \dot{\tilde{B}}_{e_i} = (\tilde{L} - D_{pi}) \cdot \tilde{B}_{e_i} + \bar{B}_{e_i} \cdot (\tilde{L}^c - D_{pi}) \]  
(3.16)

For derivations of these evolution equations, see Appendix A.

The plastic deformation rate tensors \( D_{pi} \), are related to the deviatoric stresses \( \sigma_{s_i}^d \) by a non-Newtonian flow rule with modified Eyring viscosities \( \eta_i[6] \).

\[ D_{pi} = \frac{\sigma_{s_i}^d}{2\eta_i(\bar{\tau}, p, T, S)} = \frac{G_i}{2\eta_i} \tilde{B}_{e_i}^d \]  
(3.17)

The equivalent stress is represented by \( \bar{\tau} \), \( p \) is the hydrostatic pressure, \( T \) the temperature and \( S \) the intrinsic softening. The viscosities are described by an Eyring flow rule. In order to take pressure dependence \( \mu \) and intrinsic strain softening \( S \) into account, the flow rule is adapted by Govaert et al. [6].

\[ \eta_i = \eta_0 \exp \left[ \frac{AH}{RT} + \frac{\mu p}{\bar{\tau}_0} + S \right] \frac{\bar{\tau}}{\sinh(\bar{\tau} / \bar{\tau}_0)} \]  
(3.18)
This can be rewritten for high values of $\tau$, using $\sinh(x) \approx \frac{1}{2} \exp(x)$ for large values of $x$.

$$
\eta_i = 2\eta_0 \exp\left[\frac{\Delta H}{RT} + \frac{\mu p}{\tau_0} + S\right] \frac{\tau}{\tau_0} \exp\left[-\frac{\tau}{\tau_0}\right] 
$$

(3.19)

The equivalent stress $\tau$ and hydrostatic pressure are defined according to

$$
\tau = \sqrt{\frac{1}{2} \sigma_s^d : \sigma_s^d} \quad \text{and} \quad p = -\frac{1}{3} \text{tr}(\sigma)
$$

(3.20)

In Equations 3.18 and 3.19, $\eta_0$ are the initial viscosities, $\Delta H$ the activation energy, $R$ the universal gas constant, $T$ the temperature and $\tau_0$ the characteristic stress.

The evolution of $S$ is inversely related to the evolution of plastic strain $\dot{\gamma}_p$.

$$
\dot{S} = -\frac{S}{S_0} \dot{\gamma}_p \quad \text{where} \quad S \in [S_0, 0]
$$

(3.21)

Integration of Equation 3.21 and a constant $\dot{\gamma}_p$ gives

$$
S(\tau_p) = S_0 \exp\left(-\frac{\tau_p}{\gamma_0}\right) = S_0 \cdot R(\tau_p)
$$

(3.22)

$S_0$ denotes the initial age of the material and $\dot{\gamma}_p$ the equivalent plastic strain rate. This rate is coupled to the mode with the highest initial viscosity, because this mode describes the macroscopic yield point. Since this specific mode deviates from the other modes it is from now on denoted as mode 1, so $i$ is 1. The equivalent plastic strain rate is then defined as

$$
\dot{\gamma}_p = \frac{\tau_i}{\eta_i} \quad \text{where} \quad \tau_i = \sqrt{\frac{1}{2} \sigma_{s_i}^d : \sigma_{s_i}^d}
$$

(3.23)

Klompen [4] applied a fitting to $R(\tau_p)$ on a normalized softening as function of plastic strain, using a modified Carreau-Yassuda function with $r_0$, $r_1$ and $r_2$ as fitting parameters.

$$
R(\tau_p) = \left(1 + (r_0 \cdot \exp(\tau_p))^{\frac{r_1}{r_2}}\right)^{\frac{r_2}{r_1}}
$$

(3.24)

For simplicity and in order to compare the different parameters in a better way, only one mode is taken in account for the simulations.
To compare the different parameters, one reference set is chosen with a poison ratio, $\nu$, of 0.45 and an elasticity modulus, $E$, of 500 MPa. This results in the following reference set of parameters:

<table>
<thead>
<tr>
<th>$G$</th>
<th>$\kappa$</th>
<th>$\eta_0$</th>
<th>$\mu$</th>
<th>$\tau_0$</th>
<th>$r_0$</th>
<th>$r_1$</th>
<th>$r_2$</th>
<th>$S_0$</th>
<th>$G_r$</th>
</tr>
</thead>
<tbody>
<tr>
<td>172</td>
<td>1667</td>
<td>$2.37 \times 10^{11}$</td>
<td>0.08</td>
<td>0.7</td>
<td>0.965</td>
<td>50</td>
<td>-5</td>
<td>27.0</td>
<td>26</td>
</tr>
<tr>
<td>[MPa]</td>
<td>[MPa]</td>
<td>[MPa s]</td>
<td>-</td>
<td>[MPa]</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>[MPa]</td>
<td></td>
</tr>
</tbody>
</table>

### 3.2 The inclusion material

The inclusion are made out of elastomers, these are polymers showing non-linear elastic stress-strain behavior. Elastomers are often used to refer to materials which show a rubber like behavior, even though no rubbers exist which show a purely elastic behavior.

Elastomeric materials are elastic in the classical sense. Upon unloading, the stress-strain curve is retraced and there is no permanent deformation. Figure 3.3 shows a typical stress-strain curve for an elastomeric material.

![Figure 3.3 Typical stress-strain curve of an elastomer.](image)

Calculations of stresses in elastomeric material are derived from the existence of a strain energy function. For a perfectly elastic solid at equilibrium, the stress can only be a function of the change in the internal energy $U$ due to the deformation of the material away from its reference state.
\[ \sigma = \rho \frac{\partial U}{\partial B} \]  

(3.25)

Normally, the strain energy function, \( W \), is defined as

\[ W = \rho_0 U \]  

(3.26)

For an incompressible, isotropic material equation 3.25 becomes

\[ \sigma = -pI + 2 \frac{\partial W}{\partial I_B} B - 2 \frac{\partial W}{\partial \Pi_B} B^{-1} \]  

(3.27)

Here the material function is a derivative of the strain energy function with respect to the invariants, \( I_B \) and \( \Pi_B \), of \( B \), the Finger tensor. A simplification of the strain energy is function is

\[ W = \frac{1}{2} G I_B \]  

(3.28)

Equation 3.27 becomes then

\[ \sigma = -pI + GB \]  

(3.29)

This equation was first derived by Rivlin[7] in 1948. This model is called the neo-Hookean model with \( G \) as the elastic modulus in shear. This constant can be a function of the deformation, but in this simple case we assume it will remain constant.

In the simulations a shear modules of 4 MPa is used, with a variation into 2 MPa and 8 MPa. With these low values, the rubber is much softer as the polymer matrix.
Chapter 4

Results

In order to understand the stress-strain behavior of a TPE, simulations are carried out using the finite element package Marc/Mentat. First some simple one element simulations of the thermoplastic polymer are performed to get some knowledge of the properties of this material. The next step is the simulation of the 2D RVE in various conditions. In Chapter 5 these result are compared with other software packages like Abaqus/CAE and Digimat.

4.1 One element simulations

In these simulations a homogenous deformation on a 2D plane strain element is performed (See Figure 4.1). The displacement of the right side of the element is prescribed. The strains are displayed in engineering strains. Because the length of the element is chosen 1, the displacement of the right side is also the strain. The stresses are also displayed in engineering stresses. The force to accomplish the prescribed displacement is measured and because the initial area of cross section is also 1, this force is the same as the engineering stress. All the parameters mentioned in paragraph 3.1 are varied over a certain reasonable range.

First the influence of the elasticity modulus, $E$, has been researched. In the material model this modulus is controlled by the shear modulus and the bulk modulus. With a constant Poisson ratio of 0.45 these moduli have to be adopted to obtain the appropriate E-modulus. See Eq. 4.1 and 4.2 for the relations between these four properties.
\[ G = \frac{E}{2(1 + \nu)} \quad (4.1) \]

\[ k = \frac{E}{3(1 - 2\nu)} \quad (4.2) \]

In Figure 4.2a can be seen that as expected \( E \) influences the linear elastic part before yielding. Also can be concluded that with a lower modulus the yield stress increases, while the influence on the hardening is almost zero. The increase of the yield is because the material yields at a higher strain, due to a less steeper slope of the elastic part. At this higher strain, the contribution of the hardening part is higher (See Fig. 3.2a). This hardening part is controlled only by the hardening modulus, \( G_r \), as can be seen in Figure 4.2b. This result can also be projected backwards to Equation 3.14, with \( G_r \) as the only independent variable. One can also see a slight increase of the yield point with increasing hardening modulus. The pressure dependence parameter, \( \mu \) (Figure 4.2c), defines together with the characteristic stress, \( \tau_0 \), (4.2d) and the initial softening value, \( S_0 \), (4.2e) for a large part the yield point.

A difference is that at large strains (above 50%), \( \mu \) and \( \tau_0 \) do influence this hardening part while \( S_0 \) only influence the softening. An increase of 1.0 in \( S_0 \) comes down to an increase of the yield point of about 1.40 MPa. Also the expected increase of softening can be seen in figure 4.2e. The characteristic stress also influences the softening, but this can be contributed to an overall shift of the driving stress, \( \sigma_s \), with a same elastic behavior. An increase of 0.2 MPa of \( \tau_0 \) means an overall increase of the driving stress of 20 MPa. (So also the yield point increases with 20 MPa.) This is also the reason why in Figure 4.2d at large strains this shift remains visible, in contrary to Figure 4.2e. This shift can also be seen in Figure 4.2c, in this case a decrease of \( \mu \) of 0.04 comes down to an increase of the overall driving stress of approximately 3 MPa.

As expected, \( r_0, r_1 \) and \( r_2 \) influences only the softening with almost no shift in yield point as can be seen in the Figures 4.2f, g and h. A strange thing that attracts attention in Figure 4.2f is the plot of the parameter value \( r_0 = 0.8 \), after the yield point this plot first shows hardening, then it softens at a some kind of second ‘yield’ point, and eventually it hardens in a normal way. A possible explanation for this strange behavior is that \( r_0 = 0.8 \) is beyond the validated region of this material model.
Figure 4.2 Parameter variations in single element simulations of a thermoplastic polymer

a) Stress (MPa) vs. Strain [-]

- $E = 1000$ MPa
- $E = 500$ MPa
- $E = 250$ MPa

b) Stress (MPa) vs. Strain [-]

- $G_r = 20$ MPa
- $G_r = 26$ MPa
- $G_r = 30$ MPa

c) Stress (MPa) vs. Strain [-]

- $r_0 = 0.5$ MPa
- $r_0 = 0.7$ MPa
- $r_0 = 0.9$ MPa

d) Stress (MPa) vs. Strain [-]

- $r_0 = 0.8$
- $r_0 = 0.965$
- $r_0 = 1.1$

e) Stress (MPa) vs. Strain [-]

- $r_1 = 10$
- $r_1 = 50$
- $r_1 = 90$

f) Stress (MPa) vs. Strain [-]

- $E = 1000$ MPa
- $E = 500$ MPa
- $E = 250$ MPa

g) Stress (MPa) vs. Strain [-]

- $r_2 = -5$
- $r_2 = -3$
- $r_2 = -1$
4.2 2D RVE simulations

The next step is to study the influence of the parameters of the thermoplastic material model in the 2D RVE model of an RVE. This means that the configuration of the volume element has to be chosen in such a way that it simulates real life. Either, for simplicity reasons, a simple configuration is chosen with one center sphere and four quarters of spheres at corners (See Figure 4.3a and b). With a volume percentage of 50% elastomeric inclusions, a lot of configurations are possible. The reason why the one is chosen in Figure 4.3a will be explained later in this chapter. With a 70% percentage a lot less configurations are possible (with a center sphere and four quarters) and their results don’t differ that much as for 50%. The stresses and strains are displayed in engineering values. For the modeling of the RVE, see Chapter 2.2. If not otherwise is mentioned, the inclusions have a shear modulus of 4 MPa.

![Configuration with 50% volume percentage of elastomeric inclusions](image_a)

![Configuration with 70% volume percentage of elastomeric inclusions](image_b)

**Figure 4.3a** Configuration with 50% volume percentage of elastomeric inclusions  
**Figure 4.3b** with 70% volume percentage of elastomeric inclusions

4.2.1 Interpretation of the results

The RVE behavior is studied in a repetitive tensile test, this means that the RVE first is stretched out to a 10% strain. At this point the load is released; the RVE shrinks back until the reaction force is zero. Then it’s again stretched out to 10%, then two times out to 20% strain and then two times out to 30%, every time with the load release. Due to these large deformations the use of Quad8 elements is necessary. In Figure 4.4a a significant difference is shown between Quad4 and Quad8 elements. Because Quad8 elements have 4 extra integration points, these elements are more accurate.

Another important issue is the element size. The behavior with 764 elements or 3056 elements is almost exactly the same. (See Figure 4.4b) This means that for the normal repetitive tensile simulations a number of elements of 25 to 30 along the boundary of the
RVE is accurate enough. Only in case of extreme large deformations, for instance a 100% strain, one should consider to increase these values.

The number of inclusions is also of influence in the RVE behavior. Either, the configuration has been chosen as can be seen in Figure 4.3. With more inclusions, there will be more gaps with large deformations, this means that the elements have to be smaller and thus more elements are needed. This influence the calculation time of the simulations dramatically. The influence of more inclusions can be a subject for a next study.

4.2.2 Parameters

For $\tau_0$ a similar behavior can be seen in the RVE simulations as in the one-element simulations. The elastic range is extended with an increasing $\tau_0$. After this extension the behavior isn’t influenced by this parameter anymore, even the hysteresis is the same. An issue that attracts attention is the softening in the first cycle to 20% strain. With a $\tau_0$ of 0.5 MPa this softening is gone in the overall behavior. This doesn’t mean that no material reached softening during the tensile test.

Also with the softening value, $S_0$, a similar behavior is shown as with $\tau_0$. This was also the case with the one-element simulations. Now the overall softening behavior vanishes with a $S_0$ of 20.0.

In Figure 4.5b it can be seen that the influence of $G_r$, the hardening modulus, becomes larger with higher strains. Interesting to see is that for the different values the return point at the $\sigma = 0$ MPa is exactly the same. The strain at which softening occurs is also the same. This is not the case in Figure 4.5c. For higher values of $\mu$, the strain at which overall softening occurs is lower than for lower values. The amount of softening remains constant.

![Figure 4.4a) Stress-strain behavior varied with element type b) varied with the number of elements](image)
Figure 4.5 Parameter variations in RVE simulations of a TPE

Figure 4.5e displays variations of the G modulus of the elastomeric inclusions. This shows expected behavior, because we see an overall stiffer curve at higher moduli. Interesting is again the small softening behavior that can be seen at $G = 4$ MPa and $G = 8$ MPa.
4.2.3 Softening vs. No Softening

An important material parameter is the initial softening value, \( S_0 \). Figure 4.6a shows a one element tensile test for various parameter sets. To eliminate the softening from the material model, this parameter is set to 0.001. This results in a decrease of the yield stress, as can be seen by the dotted line in Figure 4.6a. To increase this stress to the original point, the characteristic stress, \( \tau_0 \), can be increased to 1.58 MPa. (See the dashed line in Figure 4.6a.) The influence of this step to the repetitive tensile test is shown in Figure 4.6b. We see that with no softening and the high \( \tau_0 \), the hysteresis is almost zero. Also the dotted line in Figure 4.6b shows a decrease of the yield stress; this phenomenon was also displayed earlier at the one-element simulations and the RVE tests.

In Figure 4.7 the influence of 2 material parameters, \( G_r \) and \( \mu \), is evaluated. At small strains this influence is not significant; from about 10% strain they influence the stress strain behavior. For \( G_r \) this influence is even a bit larger than for \( \mu \).
4.2.4 Influence of configuration

For an RVE with a 50% volume percentage of elastomeric inclusions, there are many options possible considering the positions of the spheres. Even if is chosen for the four quarters and one sphere in the center as mentioned earlier. Variations are possible in the radii of the spheres and the center point of the sphere in the middle. Figure 4.8 shows some result of various simulations. In 4.8a the influence of the radii of both spheres is evaluated. The blue curve shows the behavior when $R_1$, the radius of the corner spheres, is almost 2 times $R_2$. This behavior differs significant from the results when all spheres are of equal size. Also the position of the center point of the middle spheres results in a different behavior. This is also the reason why the dashed curve doesn’t complete the whole cycle in the tensile test. The gap between the two spheres is so small, that extreme deformations in this area occur. An option is to adapt locally the element mesh to handle these deformations. In the real material the inclusions are also random distributed, conclusion is that a large different in radii and an off-centre center point of the middle sphere is the best configuration to simulate the repetitive RVE tensile test (Only valid with the simple configuration of the four quarters and one middle sphere).

Another configurations issue that is evaluated is a shift of the complete RVE to a certain direction. This means that the center points of the quarter spheres don’t lay on top anymore of the corner points of the RVE. In the case investigated the RVE was shifted by (-0.1,-0.1) units. The shifted RVE and the results are displayed in Figures 4.9 and 4.10. The two RVE’s are in fact the same, because of the tyings and the mutual relations which are the same. The deformed images, shown in Figure 4.10, are exactly the same if the shift is considered. The difference in the behavior curves can be explained due to a different proportion between matrix and inclusions material along the boundaries of the RVE.
Figure 4.9 Difference in stress-strain behavior of a “normal” RVE and a “shifted” RVE

Figure 4.10 Deformation images of a “normal” RVE and a “shifted” RVE
4.2.5 Other results

In this paragraph some other results will be evaluated. Figure 4.11a shows a plot of a 100% tensile straining of a RVE with 70% volume percentage elastomeric inclusions. When the softening is implemented in the material model of the polymer, the curve shows two softening points, a small one at approximately 20% strain and a large one at 90%. In Figure 4.11b the stress distribution of the first softening event is displayed. The highest stress at this moment in the polymer matrix is at this moment 60 MPa. (The lighted parts) This is below the yield stress measured in the one-element simulations. The stress distribution at 90% is shown in Figure 4.11c. In this state the highest stress in the matrix is 172 MPa.

![Figure 4.11 Results of a tensile test with 100% strain](image)

Figure 4.12 shows the behavior at different volume percentages of elastomeric inclusions. The amount of elastomers in the material is an indicator of the stiffness. A decrease of 10% volume percentage means an increase of the yield stress of approximately 50%. The stiffness of the material can be controlled in three ways by adjusting the volume percentage, the G modulus of the inclusions or the E modulus of the matrix material.

![Figure 4.12 Variation in volume percentage](image)
Chapter 5

Comparison with Digimat/Abaqus

5.1 One element

In this chapter some previous results will be compared to the result of another simulation package called Digimat. This is a nonlinear multi-scale composite materials and structures modeling platform. A part of this package is Digimat-MF (Mean Field Homogenization). This software can predict the nonlinear constitutive behavior of multiphase composite materials. In June 2008 the developers of Digimat, introduced as new material option, the Leonov formulation based on the Eindhoven model introduced by Klompen [4]. The developers made some adjustments based on a report of J.C. Simo [1992]. [9,10]

The plastic flowrule was rewritten to:

\[-\frac{1}{2} B_e B^e = \dot{\gamma} \frac{\partial f}{\partial \tau} = \dot{\varepsilon}_p \quad \text{with} \quad B_e = F \frac{d}{dt} \left( C^{-1}_p \right) F^T \]  

(5.1)

The plastic flowrule was rewritten to:

\[-\frac{1}{2} B_e B_e^e = \dot{\gamma} \frac{\partial f}{\partial \tau} = \dot{\varepsilon}_p \quad \text{with} \quad B_e = F \frac{d}{dt} \left( C^{-1}_p \right) F^T \]  

The plastic strain rate is not the material time derivative of \( \varepsilon_p = \frac{1}{2} (C_p - \delta) \).

The accumulated plastic strain rate is defined as:

\[ \dot{\gamma} = \sqrt{\frac{2}{3} \dot{\varepsilon}_p : \dot{\varepsilon}_p} \]  

(5.2)

Also they introduced an extra neo-Hookean stress according to:

\[ \tau = J\sigma = \tau^{\text{neo}} + \tau^d \quad \text{with} \quad \tau^{\text{neo}} = kJ(J-1)\delta + G_p J^{-\frac{1}{p}} B^d \quad \text{and} \quad \tau^d = GJ^{\frac{1}{p}} B^d \]  

(5.3)

Figure 5.1 single element tensile simulation a) with softening b) without softening
Simulations done by the developers of Digimat showed two problems. At first, their model did not describe the pre-yield stress-strain behavior accurately, due to their single mode approach. Secondly, the softening doesn’t match the Marc implementation of TU/e that is considered the reference. This is due the fact that they described the hardening stress by a Neo-Hookean relation in Kirchhoff stresses, introducing a factor of J, the volume change ratio, that is not present in the Eindhoven formulation.

In Figure 5.1a some one-element simulation results are shown of a EGP material. The Digimat material does match the Marc result in the pre-yield region because both are a single-mode simulation. In the softening region a difference occurs, this is as expected due to the difference in material model. When the softening is not switched on in both the material models, Marc and Digimat we see a better match, almost exactly the same, as can be seen in Figure 5.1b. After yield there occurs some difference, this is due to the decomposition of \( \tau \).

Another software package that implemented the Leonov model as a material is Abaqus. Because of some adoptions and maybe wrong interpretation of the parameters this results doesn’t match the Marc results. This can be seen in Figure 5.1a. It seems that the shift occurs due to an error in the applied strain rate. The reasons why this occurs are not a subject of this report and could be investigated in a further study.

5.2 2D RVE

For a comparison between the RVE stress-strain behavior of a TPE model (without softening) in Marc and in Digimat, the Digimat material is loaded into Abaqus and the same cyclic tensile test as in Chapter 4 is simulated. The result is shown in Figure 5.2. As one can clearly see, the results match perfectly. Also the stress distributions are almost exactly the same as is shown in Figure 5.3a for the Marc simulation and Figure 5.3b for the Abaqus/Digimat simulation. For instance, the location of the parts between 68 and 45 MPa (yellow and light orange) in the Marc result compares with the location of the orange part in the Abaqus result, between 71 and 49 MPa. Only difference is the more extreme result in Figure 5.3b.

Figure 5.2 Comparison between Marc/Mentat and Abaqus/Digimat
In this section we briefly discuss 3D RVE’s generated by Digimat FE and the comparison with Digimat MF. As mentioned before, Digimat MF performs a mean field homogenization of multi-phase materials, so that it can be treated as a material with one set of parameters. Digimat FE is a software program that creates a 3D RVE structure. Many options are available, such as the volume percentage, shape and orientation of the inclusions. To compare the results of Digimat MF with a 3D RVE, an RVE is taken with an inclusion percentage of 50%. The inclusions have a spherical shape with random radius between 0 and 0.25. A snapshot of the 3D RVE is displayed in Figure 5.5 at the left. In the simulation the 3D RVE doesn’t act like a “real” RVE, as used in the Marc simulations. The RVE’s created by Digimat FE don’t have periodic boundary conditions. Only the nodes on every boundary face are tied to a corresponding point in space with the

Figure 5.3 Comparisons between Marc/Mentat(top) and Abaqus/Digimat(bottom)

5.3 3D RVE

In this section we briefly discuss 3D RVE’s generated by Digimat FE and the comparison with Digimat MF. As mentioned before, Digimat MF performs a mean field homogenization of multi-phase materials, so that it can be treated as a material with one set of parameters. Digimat FE is a software program that creates a 3D RVE structure. Many options are available, such as the volume percentage, shape and orientation of the inclusions. To compare the results of Digimat MF with a 3D RVE, an RVE is taken with an inclusion percentage of 50%. The inclusions have a spherical shape with random radius between 0 and 0.25. A snapshot of the 3D RVE is displayed in Figure 5.5 at the left. In the simulation the 3D RVE doesn’t act like a “real” RVE, as used in the Marc simulations. The RVE’s created by Digimat FE don’t have periodic boundary conditions. Only the nodes on every boundary face are tied to a corresponding point in space with the
result that every boundary face stays flat. Therefore the boundary face doesn’t curve as in Figure 5.3 with the curved edges.

Figure 5.4 shows the result of simple tensile test in plane stress conditions, because Digimat MF only can calculate with this condition. This is different from the 2D simulations, which are performed in plane strain conditions. The difference in the two curves is significant. The expectation is that if the number of inclusions is increased to infinity the two curves must lie on top of each other. To investigate this, there is a lot more research required.

![Figure 5.4 Stress-strain curve of a TPE RVE calculated with Digimat MF and Abaqus/Digimat](image)

**Figure 5.4 Stress-strain curve of a TPE RVE calculated with Digimat MF and Abaqus/Digimat**

![Figure 5.5 Examples of 3D RVE’s with strain = 0% (left) and Strain = 50% (right)](image)

**Figure 5.5 Examples of 3D RVE’s with strain = 0% (left) and Strain = 50% (right)**
Chapter 6

Conclusion and Recommendations

- The material model as developed by Klompen [4], Den Hartog[2] and Breemen[9] could be a basis for reverse engineering with results of tensile experiments. With this reverse engineering the model parameters of the experimented material could be extracted.

- For the simplicity and understanding of the research some assumptions are made, such as the use of the single-mode in the EGP material model, instead of multi-mode. Further research has to be conducted to investigate the stress-strain behavior without these assumptions.

- The Abaqus implementation of the EGP model was not in a state, that it was useful to be a full subject to investigate. For later studies on TPE, this implementation could be very useful.

- The software package Digimat is a powerful tool to predict the behavior of multi-phase materials, in 2D as in 3D. In order to give a good consideration about the results more research is required.

- The 3D RVE’s generated by Digimat FE aren’t “real”, because they don’t have the proper periodic boundary conditions. To compare the 3D with the 2D results, the boundary faces of the 3D RVE should be tied together in a similar way as in 2D. This is a complex matter and is interesting for further research.
Bibliography


[8] Marc user manuals A, B, C and D


Appendix A

Derivations of the evolution equations

Derivation of the volume factor rate, see Equation 3.15

\[ \dot{J} = \det (F) \dot{F}^{-1} : \dot{F} \]  
\[ = \text{Jtr}(\dot{F} : \dot{F}^{-1}) \]  
\[ = \text{Jtr}(L) = \text{Jtr}(D) \]  
\[ (A.1) \]
\[ (A.2) \]
\[ (A.3) \]

Derivation of the elastic strain rate. This derivation can be applied to all modes, see Equation 3.15

\[ \tilde{B}_e = \tilde{F}_e \cdot \tilde{F}_e^c \]  
\[ \tilde{\dot{B}}_e = \tilde{F}_e \cdot \tilde{F}_e^c + \tilde{F}_e \cdot \tilde{\dot{F}}_e^c \]  
\[ \tilde{\dot{F}}_e = \tilde{F} \cdot F_p^{-1} \]  
\[ \tilde{\dot{F}}_e = \tilde{\dot{F}} \cdot F_p^{-1} + \tilde{F} \cdot \tilde{F}_p^{-1} \]  
\[ F_p \cdot \tilde{\dot{F}}_p^{-1} = -\dot{F}_p \cdot F_p^{-1} \]  
\[ (A.4) \]
\[ (A.5) \]
\[ (A.6) \]
\[ (A.7) \]
\[ (A.8) \]

Substitution of Equations 3.6, 3.8 and the ones mentioned above into Equation A.5 for \( \tilde{B}_e \) results in the following equation.

\[ \tilde{\dot{B}}_e = \left( \tilde{\dot{F}} \cdot F_p^{-1} + \tilde{F} \cdot \tilde{F}_p^{-1} \right) \cdot \tilde{F}_e^c + \tilde{F}_e \cdot \left( F_p^{-c} \cdot \tilde{F}_e^c + \tilde{F}_p^{-c} \cdot \tilde{F}_e^c \right) \]  
\[ = \left( \tilde{\dot{F}} \cdot F_p^{-1} \cdot \tilde{F}_e^c + \tilde{F} \cdot \tilde{F}_p^{-1} \cdot \tilde{F}_e^c \right) \cdot B_e + \tilde{B}_e \cdot \left( F_p^{-c} \cdot \tilde{F}_e^c + \tilde{F}_p^{-c} \cdot \tilde{F}_e^c \cdot \tilde{F}_e^c \right) \]  
\[ = \left( \tilde{L} + \tilde{F}_e \cdot F_p^{-1} \cdot \tilde{F}_e^c \right) \cdot B_e + \tilde{B}_e \cdot \left( \tilde{L} + F_p^{-c} \cdot \tilde{F}_p^{-c} \cdot \tilde{F}_e^c \right) \]  
\[ = \left( \tilde{L} - D_p \right) \cdot B_e + \tilde{B}_e \cdot \left( \tilde{L} - D_p \right) \]  
\[ (A.9) \]
\[ (A.10) \]
\[ (A.11) \]
\[ (A.12) \]