A constitutive model for polymers: Formulation and Integration algorithm

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Mestrado em Engenharia Matemática
Departamento de Matemática
2014

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Todas as correções determinadas pelo júri, e só essas, foram efetuadas.

O Presidente do Júri,

Porto, _____/_____/______
Dedicated to my husband ...
Acknowledgements

I would like to gratefully acknowledge Prof. Pires for accepting to be my thesis supervisor and letting me integrate is his research group. I would also like to thank Prof. Gama for being my thesis co-supervisor and his support during accomplishment of this work. Eng. Mirkhalaf, a PhD student from research group of Prof. Pires, helped me to get acquainted with concepts of continuum mechanics and Finite Element Method and also constitutive modelling of polymers. I am grateful for his support and his comments while I was involved in my thesis.
Being far from my country has been difficult and my friends company has been helping me to keep moving. I thank them all although I can not name all of them.
At last, not the least, I am going to deeply thank my husband and my family for their undeniable support without which my studies could be much harder to finish.
Abstract

The objective of this thesis is to develop an elasto-viscoplastic constitutive model in order to characterize the deformation behaviour of polymeric materials. More importantly, it is intended to incorporate several numerical techniques to solve the equilibrium equation obtained from kinematic and material constitutive relations. For this purpose, the thesis starts with a global overview of the state-of-art on the present topic in Chapter 1. In Chapter 2, the main concepts of the Continuum Mechanics Theory and the Finite Element Method are briefly reviewed. This chapter is followed by development of the BPA based constitutive model in Chapter 3. In Chapter 4, the most important contribution of this work is introduced, which is derivation of the integration algorithm and finite element implementation of the model. In order to assess the capability of the model to predict the typical deformation behaviour of polymeric materials and the efficiency of the integration algorithm and the code, some numerical examples are provide in Chapter 5. The document finishes with the presentation of the main conclusions of this work in Chapter 6 and, in addition, suggestions for future research are made.
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Chapter 1

Introduction

1.1 General introduction

Polymers are a group of materials which, from a microscopic point of view, contain a large number of structural units linked together by the same kind of joints. Chain like structures are often observed in these substances. It can be claimed that form the beginning of time polymers have existed in the natural world. Artificial or man-made polymers have been under study from 1832. Amazingly, the polymer industry nowadays is larger than the combination of aluminum, copper and steel industries.

Polymers are a group of materials which have remarkable attractive qualities form processability to mechanical and thermal properties. Therefore, although they have not been introduced for a long time (from the beginning of 18th century), polymers are being widely used in structures and other applications. It is worth noting that despite the widespread use of polymers, their mechanical behavior is not yet thoroughly understood.

Polymers have a variety of applications that are far more than any other class of materials existing for mankind. The vast area of applications includes adhesives, coatings, foams, and packaging materials to textile and industrial fibers, composites, electronic devices, bio-medical devices, optical devices, and precursors used for high-tech ceramics which have been recently developed.
1.2 Modeling of the mechanical behavior of polymers

During the last few decades, many researchers have devoted their work to develop constitutive models for different materials such as metals and polymers. A constitutive model could be briefly defined as a set of mathematical relations which determine the relation between applied forces and displacements of any single point of the body under study. Here, we provide a very brief summary of the most well established constitutive models proposed for polymers through the last decades.

The usage of polymers is increasing in different structures. Hence, the academic community has dedicated remarkable effort to the development of constitutive models capable of characterizing the behavior of polymers. It can be said that the initiation of the efforts to determine the behavior of polymers dates back to 1930s. Eyring (1936) proposed a molecular theory for the yield stress of amorphous polymers, considering the yield behavior as a thermally activated process. Temperature and strain rate effect is accounted for in the theory. Mooney (1940) proposed a strain energy function for rubber elastic materials. Haward and Tackray (1968) developed a one-dimensional constitutive model for glassy polymers. The work could be considered as the first constitutive model proposed for predicting the deformation behavior of glassy polymers. The three dimensional version of Haward and Tackray model was proposed by Boyce et al. (1988). A modified version of this model was later formulated by Wu and van der Giessen (1994). The other constitutive model which is able to predict the typical deformation behavior of polymeric materials is the generalised compressible Leonov model, which has been proposed by Baaijens (1991) and extended by Tervoort et al. (1998) and Govaert et al. (2000). For a review on finite element simulation of polymers, the reader is referred to Mackerle (1997) and Mackerle (2003). The phenomenological constitutive models developed for amorphous polymers could be, in many cases, used for semi-crystalline polymers as well. The molecular orientation of polymers evolves during large deformations and the corresponding strengthening is, for some polymers, greatly dependent on strain state. Time dependent deformation and failure of polymers have been studied using linear and non-linear visco-elastic and visco-plastic FEM models (Mackerle (1997); Mackerle (2003)).

1.3 Scope and outline

The aims of the work can be expressed as follows:
• To study the non-linear continuum solid mechanics theory;

• To study non-linear finite element method (FEM);

• To develop a constitutive model based on BPA (Mary C. Boyce, David M. Parks, Ali S. Argon) model (Boyce et al., 1988);

• To use nonlinear finite element method to solve the equilibrium equations obtained from continuum mechanics relations and the constitutive model;

• To derive the integration algorithm of the model developed in the previous section in order to be used in finite element;

• To run numerical examples with the implemented model within finite element.

In the next chapter of the work, continuum mechanics and finite element method are explained. It should be mentioned that the objective is by no means providing a comprehensive review of the subjects and it is intended to provide the main relations which are used in this work. In Chapter 3, the analytical formulation of the model based on BPA model is provided. The numerical treatment of the governing constitutive equations and the integration algorithm of the model which includes the derivation of state update procedure and also consistent tangent operator, is given in Chapter 4. Some numerical examples are conducted using the implemented constitutive model in Chapter 5. Finally, in Chapter 6, the results and conclusions of this work are presented.
Chapter 2

Continuum mechanics and finite element method

In order to characterize the behaviour of polymeric materials, we need to either develop new constitutive models or use some existing models capable of predicting typical behaviour of polymers. Before developing or using any constitutive model, it is required to be familiarized with basic concepts of standard continuum mechanics. Once the basic continuum mechanics is learned, a suitable numerical approach is needed in order to solve the equilibrium equation obtained from continuum mechanics. In this work, finite element method (FEM) is used for solution of equilibrium problem for solid polymeric materials.

2.1 Continuum Mechanics

The concepts of continuum mechanics are presented in this section. In order to have a more comprehensive description of the topic, you can refer to Shabana (2008), Criesfield (2000), Holzapfel (2000).

2.1.1 Kinematics of deformation

In this section, motion of particle, the definition of deformation gradient, different strain measures, the velocity gradient and different stress measures are explained.

2.1.1.1 Motion

p is a particle of a body $\Omega_0$. The body is limited to its boundary $\partial \Omega_0$. A motion $\varphi$ applies to the body and after application of the motion the particle $P$ has a new
position \( x \). The new position is function of time \( t \) as well.

\[
x = \varphi(p, t).
\]  

(2.1)

From the new position of the particle to the original position, a displacement field is given by:

\[
u(p, t) = \varphi(p, t) - p.
\]  

(2.2)

If we assume that the motion \( \varphi \) is invertible, relation (2.3) can be written:

\[
p = \varphi^{-1}(x, t).
\]  

(2.3)

According to above mentioned equations, two different configurations are being assumed. The initial configuration (undeformed configuration or material configuration) in which the particle \( p \) exists. The other configuration is current configuration (deformed configuration or spatial configuration).

In order to obtain the velocity of particle \( p \), relation (2.4) could be used.

\[
dx = \frac{\partial \varphi(p, t)}{\partial t},
\]  

(2.4)

Using relations (2.3) and (2.4), one can write:

\[
v(x, t) = \dot{x}(\varphi^{-1}(x, t), t),
\]  

(2.5)

which is the velocity of the material particle \( x \) at time \( t \).

### 2.1.1.2 The deformation gradient

Deformation gradient is defined as the gradient of motion \( \varphi \) in order to particle \( p \):

\[
F(p, t) = \nabla_p \varphi(p, t) = \frac{\partial x_t}{\partial p}.
\]  

(2.6)

By substituting (2.2) in (2.6) we can have:

\[
F = I + \nabla_p u,
\]  

(2.7)

where \( I \) is the second order identity tensor. It should be emphasized that in relations (2.6) and (2.7), the deformation gradient is defined in the reference configuration and the operator \( \nabla_p \) is generally a material gradient operator. If it is required to have the deformation gradient in the spatial configuration, we should use spatial gradient
operator, $\nabla_x$. Equation (2.8) gives the deformation gradient at current configuration.

$$F(x, t) = [\nabla_x \varphi^{-1}(x, t)]^{-1} = [\mathbf{I} - \nabla_x \mathbf{u}]^{-1}.$$  (2.8)

The change in the volume of the body under motion is equivalent to the determinant of the deformation gradient and represented by $J$ and also called deformation Jacobian.

$$J = \det \mathbf{F}.$$  (2.9)

Polar decomposition of the deformation gradient gives:

$$\mathbf{F} = \mathbf{R} \mathbf{U} = \mathbf{V} \mathbf{R},$$  (2.10)

where $\mathbf{R}$ is a proper orthogonal tensor called rotation tensor. In relation (2.10), $\mathbf{U}$ and $\mathbf{V}$ are symmetric positive definite tensors and called right and left stretch tensors, respectively. The right and left stretch tensors are also represented as:

$$\mathbf{U} = \sqrt{\mathbf{C}}; \quad \mathbf{V} = \sqrt{\mathbf{B}},$$  (2.11)

where $\mathbf{C}$ and $\mathbf{B}$ are, respectively, right and left Cauchy-Green strain tensors defined by

$$\mathbf{C} = \mathbf{U}^2 = \mathbf{F}^T \mathbf{F}; \quad \mathbf{B} = \mathbf{V}^2 = \mathbf{F} \mathbf{F}^T.$$  (2.12)

### 2.1.1.3 Strain measures

A particle is strained when, as deformation proceeds, the relative position of the material particle changes. There are different approaches to measure the strain of a material particle. Some strain measures are used more frequently than the others due to their physical meaning and mathematical convenience.

Lagrangian strain tensor is one of the most important class of strain measures:

$$E^{(m)} = \begin{cases} \frac{1}{m} (\mathbf{U}^m - \mathbf{I}), & m \neq 0 \\ \ln[\mathbf{U}], & m = 0 \end{cases}$$  (2.13)

where, $\mathbf{U}$ is the right stretch tensor; $\mathbf{I}$ is second order identity tensor; $m$ is a real number and $\ln[\bullet]$ is tensorial logarithm. Similarly, another important family of strain
tensors, called Eulerian strain tensors, are defined by using the left stretch tensor, \( V \).

\[
\varepsilon^{(m)} = \begin{cases} 
\frac{1}{m}(V^m - I), & m \neq 0 \\
\ln|V|, & m = 0 
\end{cases}
\] (2.14)

In this work, Eulerian strain tensor is used and the logarithmic strain tensor \((m = 0)\) is considered. It is also worth noting that when the deformation is just a rotation (i.e., \( F = R \)), Eulerian strain tensor and Lagrangian strain tensor are null.

\[
U = I \implies E^{(m)} = 0, 
\] (2.15)

\[
V = I \implies \varepsilon^{(m)} = 0. 
\] (2.16)

### 2.1.1.4 The velocity gradient

Velocity gradient is defined by:

\[
L = \nabla x \mathbf{v}, 
\] (2.17)

or, alternatively by

\[
L = \dot{F}F^{-1}. 
\] (2.18)

The velocity gradient is additively composed of symmetric and skew part:

\[
L = D + W, 
\] (2.19)

where,

\[
D = \text{sym}(L) = \frac{1}{2} (L + L^T), \quad W = \text{skew}(L) = \frac{1}{2} (L - L^T). 
\] (2.20)

The symmetric part of the deformation gradient, \( D \), is called rate of deformation (stretching) tensor and the skew part, \( W \), is called spin tensor. Stretching tensor is associated with straining whereas spin tensor is associated with rigid velocities.

### 2.1.1.5 Stress measures

The Cauchy stress, \( \sigma \), the Kirchhoff stress, \( \tau \), and the first Piola-Kirchhoff stress, \( P \), are three important stress measures. Which, Cauchy stress tensor or true stress is defined as:

\[
t = \sigma n, 
\] (2.21)

where \( t \) is the surface traction and \( n \) is its associated normal vector. The Cauchy stress tensor is additively composed of hydrostatic term and deviatoric part

\[
\sigma = s + pI, 
\] (2.22)
where $s$ is the deviatory stress and $p$ is hydrostatic pressure:

$$s = dev(\sigma) = l_d : \sigma, \quad (2.23)$$

where $l_d$ is the deviatoric fourth order identity tensor:

$$l_d = l_s - \frac{1}{3}(I \otimes I), \quad (2.24)$$

where $l_s$ is the symmetric fourth order identity and $I$ is the second order identity. $l_s$ and $I$ in component form can be shown as:

$$l_{ijkl} = \frac{1}{2} [\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}], \quad (2.25)$$

$$I_{ij} = \delta_{ij}, \quad (2.26)$$

where, $\delta$ is the Kronecker delta. The hydrostatic pressure is given by:

$$p = \frac{1}{3} tr(\sigma). \quad (2.27)$$

The second stress measure is the Kirchhoff stress tensor denoted by $\tau$ defined as

$$\tau = J\sigma. \quad (2.28)$$

Similarly to the Cauchy stress, the Kirchhoff stress tensor can also be split into two parts, i.e.,

$$\tau = \tau_d + \tau_h I, \quad (2.29)$$

where $\tau_d = dev[\tau]$ and $\tau_h = \frac{1}{3} tr[\tau]$ are, respectively, the deviatoric and hydrostatic (or spherical) parts. The last stress measure mentioned here is first Piola-Kirchhoff stress tensor, denoted by $P$, also known as nominal stress. The Piola-Kirchhoff stress is defined by:

$$P = J\sigma F^{-T} = \tau F^{-T}. \quad (2.30)$$

**2.1.2 Fundamental laws**

The quantities and definitions mentioned above are essential mathematical relations of deformation. The fundamental laws of continuum mechanics governing the physical phenomena of deformation provide relations between defined and expressed quantities.
2.1.2.1 Conservation of mass

The conservation of mass postulate implies:

\[ \dot{\rho} + \text{div}_x (\rho \dot{\mathbf{u}}) = 0, \]  
(2.31)

where \( \rho \) is the density at the deformed configuration.

2.1.2.2 Momentum balance

The momentum balance, also referred to as strong form of the equilibrium equation, of any given body can be expressed as

\[ \text{div}_x \mathbf{\sigma} + \mathbf{b} = \rho \ddot{\mathbf{u}}, \]  
(2.32)

where \( \mathbf{b} \) denotes the body force vector in the deformed configuration. The equilibrium equation (2.32) needs to fulfill the following boundary condition:

\[ \mathbf{t} = \mathbf{\sigma n}, \]  
(2.33)

where \( \mathbf{t} \) is a tension vector applied on the boundary of the body.

2.1.2.3 The first and second principles of thermodynamics

The first principle of thermodynamics postulates that the energy must be conserved. This can be mathematically expressed as

\[ \rho \dot{\mathcal{E}} = \mathbf{\sigma} : \mathbf{D} + \rho r - \text{div}_x \mathbf{q}, \]  
(2.34)

where \( \mathcal{E} \), \( r \) and \( \mathbf{q} \) are, respectively, the specific internal energy, the density of heat production and the heat flux. Throughout this work, only processes with constant temperature will be considered. In this case, the first principle reduces to

\[ \rho \dot{\mathcal{E}} = \mathbf{\sigma} : \mathbf{D}. \]  
(2.35)

The equation above states that the rate of internal energy per unit deformed volume must equal the stress power, \( \mathbf{\sigma} : \mathbf{D} \), per unit deformed volume. Making use of the relation below,

\[ \tilde{\rho} = J \rho, \]  
(2.36)
where \( \bar{\rho} \) denotes the reference density, it is possible to rewrite equation (2.35) as

\[
\bar{\rho} \dot{e} = \boldsymbol{\tau} : \mathbf{D}.
\]  

(2.37)

The second principle of thermodynamics is associated with the so-called irreversibility of entropy production, expressed by the following inequality:

\[
\rho T \dot{s} + \text{div}_x \boldsymbol{q} - \rho r \geq 0,
\]  

(2.38)

where \( s \) denotes the entropy and \( T \) is the temperature. Similar to the case of the first principle of thermodynamics, if only isothermal processes are considered, Equation (2.38) is then given by

\[
\rho T \dot{s} \geq 0.
\]  

(2.39)

Pre-multiplying the equation (2.39) by \( J \), we have

\[
\bar{\rho} T \dot{s} \geq 0.
\]  

(2.40)

2.1.2.4 The Clausius-Duhem inequality

Firstly, we introduce the Helmholtz free energy, \( \psi \), defined by

\[
\psi = e - Ts
\]  

(2.41)

Re-arranging the equation (2.41) and differentiating with respect to time, we have

\[
T \dot{s} = \dot{e} - \dot{\psi}.
\]  

(2.42)

We remark that the temperature has been assumed constant, thus, \( \dot{T} = 0 \) Using the equation (2.35), we conclude that

\[
\bar{\rho} T \dot{s} = \boldsymbol{\tau} : \mathbf{D} - \bar{\rho} \dot{\psi};
\]  

(2.43)

with

\[
\boldsymbol{\tau} : \mathbf{D} - \bar{\rho} \dot{\psi} \geq 0.
\]  

(2.44)

The fundamental inequality above is called Clausius-Duhem inequality.
2.1.3 The quasi-static initial boundary value problem

The fundamental laws presented in the last section allow us to define an initial boundary value problem (IBVP) associated with the description of a given deformation process. The solution of the IBVP delivers the prediction of how a given solid will mechanically behave when subjected to certain boundary conditions. Within the scope of this work, only quasi-static problems will be addressed, hence, all inertia effects will be neglected. Thus, the equilibrium equation (2.32), in the strong form, is re-written to be given by

\[ \text{div}\sigma = 0. \quad (2.45) \]

Multiplying the equation (2.45) by a virtual displacement, \( \eta \), and integrating over the volume, we have

\[ \int_{\varphi(\Omega)} (\text{div}\sigma)^T \eta dV = 0. \quad (2.46) \]

After some straightforward operations, (2.46) becomes

\[ \int_{\varphi(\Omega)} [\sigma : \nabla_x \eta - (\text{div}\sigma \cdot \eta)] dV = 0. \quad (2.47) \]

Making use of the divergence theorem, we have

\[ \int_{\varphi(\Omega)} \sigma : \nabla_x \eta dV - \int_{\varphi(\partial\Omega)} (\sigma \cdot n)^T \eta dA = 0. \quad (2.48) \]

Finally, substituting Equation (2.33) into Equation (2.48) leads to

\[ \int_{\varphi(\Omega)} \sigma : \nabla_x \eta dV - \int_{\varphi(\partial\Omega)} t \cdot \eta dA = 0. \quad (2.49) \]

Equation (2.49) is called weak form of the equilibrium equation. The use of the weak form can significantly facilitate the use of efficient numerical methods for the solution of the structural IBVP. With the definition of weak equilibrium at hand, we can define the quasi-static IBVP, in the spatial description, as follows.

**Problem 2.1**

Given a prescribed deformation gradient history

\[ \mathbf{F}(t) = I + \nabla_p \mathbf{u}(p, t) \quad (2.50) \]

and the Cauchy stress, at each point of the body expressed as

\[ \sigma(t) = \sigma(\mathbf{F}(t, \alpha(t))) \quad (2.51) \]
obtained from the solution of the constitutive initial boundary value problem where \( \alpha \) is the set of internal variables associated with the material, find a kinematically admissible displacement function, \( u \in \mathcal{K} \) such that the equation

\[
\int_{\varphi(\Omega)} \sigma(t) : \nabla \eta dV - \int_{\varphi(\partial\Omega)} t(t) \cdot \eta dA = 0,
\]

is satisfied for all \( t \in [t_0, t_n] \) and for all \( \eta \in \nu_t \). The set of kinematically admissible displacements, \( \mathcal{K} \), and the space of virtual displacements at time \( t \), \( \nu_t \), are respectively given by

\[
\mathcal{K} = \{ u : \Omega \rightarrow \mathcal{U} | u(p, t) = \bar{u}(p, t), t \in [t_0, t_n], p \in \partial \varphi_u \},
\]

\[
\nu_t = \{ \eta : \varphi \rightarrow \mathcal{U} | \eta = 0 \in \partial \varphi_u \}.
\]

Unfortunately, analytical solutions for the problem defined above exist only for a restricted set of special cases. For accurate predictions of the mechanical behavior of solids in the general case, the use of numerical methods is therefore indispensable.

### 2.1.3.1 The material version

For reference, the material version of the weak form of the equilibrium equation is also herein provided, which reads

\[
\int_{\varphi} P : \nabla \eta dV - \int_{\partial \varphi} \bar{t} \cdot \eta dA = 0,
\]

where \( \bar{t} \) is the surface traction per unit reference area.

### 2.2 Displacement-based finite elements

In this section, the general concepts of the finite element method formulated with a displacement-based approach will be briefly addressed. The finite element method has been chosen in this work as the base numerical tool mainly due to its versatility and its high effectiveness when adopted for the simulation of deformation processes.

#### 2.2.1 Spatial discretisation

As stressed out above, the solution of Problem 2.1 often requires the use of some sort of numerical strategy. Within a typical finite element framework, the field variables
are discretised through the so-called interpolation or shape functions. In the case of displacement-based finite elements, the interpolated field variable are the displacements. Within a given element \( e \), the interpolation is assumed to be

\[
\mathbf{u}(\mathbf{x}) = \sum_{i=1}^{n_{\text{node}}} N_i^{(e)}(\mathbf{x}) \mathbf{u}_i,
\]

(2.56)

where \( N_i^{(e)}(\mathbf{x}) \) is the shape function associated with node \( i \) (evaluated at \( \mathbf{x} \)) and \( n_{\text{node}} \) is the number of nodes of the element. In similar manner, a global interpolation function can also be set, that is,

\[
\mathbf{u}(\mathbf{x}) = \sum_{i=1}^{n_{\text{poin}}} N_i^{g}(\mathbf{x}) \mathbf{u}_i,
\]

(2.57)

where \( n_{\text{poin}} \) is the total number of nodes of the finite element mesh and \( N_i^{g}(\mathbf{x}) \) is the global interpolation matrix which can be represented by

\[
\mathbf{N}^g(\mathbf{x}) = \left[ \text{diag}[N_1^{g}(\mathbf{x})] \text{ diag}[N_2^{g}(\mathbf{x})] \cdots \text{ diag}[N_{n_{\text{poin}}}^{g}(\mathbf{x})] \right]
\]

(2.58)

where \( \text{diag}[N_i^{g}] \) denotes a \( n_{\text{dim}} \times n_{\text{dim}} \) diagonal matrix defined

\[
\text{diag}[N_i^{g}] = \begin{pmatrix}
0 & \cdots & 0 \\
N_i^{g} & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & N_i^{g}
\end{pmatrix}.
\]

(2.59)

At this point, it is also convenient to define the global vector of nodal displacements, given by

\[
\mathbf{u} = [u_1^1, \ldots u_1^{n_{\text{dim}}}, \ldots, u_{n_{\text{poin}}}^1, \ldots, u_{n_{\text{poin}}}^{n_{\text{dim}}}]^T.
\]

(2.60)

With the above matrix notation at hand, equation (2.55) can be rephrased to be given by

\[
\mathbf{u}(\mathbf{x}) = \mathbf{N}^g(\mathbf{x}) \mathbf{u},
\]

(2.61)

where the equation above represents the interpolation of the displacement field by means of discrete functions. Analogously, we can write the field of virtual displacements to be given by

\[
\mathbf{\eta}(\mathbf{x}) = \mathbf{N}^g(\mathbf{x}) \mathbf{\eta}.
\]

(2.62)

We also define the global discrete symmetric gradient matrix, \( \mathbf{B}^g \), which in the case of plane stress and plane strain problems assumes the form

\[
\mathbf{B}^g = \begin{pmatrix}
N_{1,1}^{g} & 0 & \cdots & N_{n_{\text{poin}},1}^{g} & 0 \\
0 & N_{1,2}^{g} & \cdots & 0 & N_{n_{\text{poin}},2}^{g} \\
N_{1,2}^{g} & N_{1,1}^{g} & \cdots & N_{n_{\text{poin}},2}^{g} & N_{n_{\text{poin}},1}^{g}
\end{pmatrix},
\]

(2.63)
where use of the following notation has been made:

\[(\cdot)_{ij} = \frac{\partial (\cdot)_{i}}{\partial x_{j}}. \quad (2.64)\]

For completeness, the global discrete full gradient operator, \( G^g \), is also provided herein, whose format in plane stress and plane strain analyses is given by

\[
G^g = \begin{pmatrix}
N^g_{1,1} & 0 & N^g_{2,1} & 0 & \cdots & N^g_{n,1} & 0 \\
0 & N^g_{1,1} & 0 & N^g_{2,1} & \cdots & 0 & N^g_{n,1} \\
N^g_{1,2} & 0 & N^g_{2,2} & 0 & \cdots & N^g_{n,2} & 0 \\
0 & N^g_{1,2} & 0 & N^g_{2,2} & \cdots & 0 & N^g_{n,2}
\end{pmatrix}. \quad (2.65)
\]

### 2.2.2 Temporal discretisation. The non-linear incremental finite element procedure

In practical engineering applications, it is often required the modeling of materials that are dependent of the deformation history. Such materials are called path dependent and, regardless whether they take strain rate effects into account or not, a suitable temporal discretisation needs to be performed. Within the context of most of this work, a pseudo-time discretisation between the time increments \([t_n, t_{n+1}]\) will be considered for which a fully implicit scheme is adopted.

For a generic path-dependent material model, an incremental constitutive function, \( \dot{\sigma} \), is assumed to exist, i.e.,

\[
\sigma_{n+1} = \dot{\sigma}(F_{n+1}, \alpha_n). \quad (2.66)
\]

In practice, the function \( \dot{\sigma} \) is associated with an integration algorithm that computes the material behavior for a given deformation gradient \( F_{n+1} \) and set of internal variables, \( \alpha_n \), which remain constant within \([t_n, t_{n+1}]\). Accordingly, a similar incremental function for the set of internal variables is also defined:

\[
\alpha_{n+1} = \dot{\alpha}(F_{n+1}, \alpha_n). \quad (2.67)
\]

Up to this point, it suffices to leave the incremental constitutive functions \( \dot{\sigma} \) and \( \dot{\alpha} \) unspecified for the sake of generality.

### The non-linear incremental finite element equation

The definition of the incremental constitutive function of Section 2.2.2, combined with the spatial discretisation presented in Section 2.2.1, allows the definition of the
2.2 Displacement-based finite elements

incremental finite element equilibrium equation, obtained after some straightforward substitutions and rearrangements from Equation (2.49):

\[ \mathbf{r}(\mathbf{u}_{n+1}) \equiv \mathbf{f}^{\text{int}}(\mathbf{u}_{n+1}) - \mathbf{f}^{\text{ext}} = 0, \]

where \( \mathbf{f}^{\text{int}} \) and \( \mathbf{f}^{\text{ext}} \) are, respectively, the internal and external force vectors, defined for a given element \( e \) as

\[ \mathbf{f}^{\text{int}} = \int_{\varphi_{n+1}(\varphi^{(e)})} \mathbf{B}^T \mathbf{\hat{\sigma}}(\mathbf{F}_{n+1}, \alpha) dV, \]  

(2.69)

\[ \mathbf{f}^{\text{ext}} = \int_{\varphi_{n+1}(\partial \varphi^{(e)})} \mathbf{N}^T \mathbf{t}_{n+1} dA, \]  

(2.70)

Within the scope of this work, Equation (2.64) will be generally non-linear and therefore requires an adequate (numerical) method for its solution. Considering an incremental scheme, in which a given fraction of the external prescribed load is applied at each increment, Equation (2.64) is solved as summarized in Box 1.

Remark 2.1.

In practice, the external force is computed by the expression

\[ \mathbf{f}^{\text{ext}}_{n+1} = \lambda_{n+1} \mathbf{\bar{f}}^{\text{ext}}, \]  

(2.71)

where \( \lambda_{n+1} \) is the prescribed load factor at time \( t_{n+1} \) and \( \mathbf{\bar{f}}^{\text{ext}} \) is computed only once at the first iteration of the incremental procedure through the expression

\[ \mathbf{\bar{f}}^{\text{ext}} = \int_{\varphi_{n+1}(\partial \Omega^{(e)})} \mathbf{N}^T \mathbf{\bar{t}} dA \]  

(2.72)

where \( \mathbf{\bar{t}} \) is a prescribed field, which remains constant through the incremental procedure.

Numerical integration of \( \mathbf{f}^{\text{int}} \) and \( \mathbf{f}^{\text{ext}} \)

One important aspect of the finite element implementation is the substitution of the exact integrals of Equations (2.69) and (2.70) by some numerical approximations. In this work, both the internal and external force vectors will be integrated using standard Gaussian quadratures. For instance, in the case of the internal force vector, \( \mathbf{f}^{\text{int}} \) is approximated by the following expression:

\[ \mathbf{f}^{\text{int}}_{(e)} = \int_{\varphi_{n+1}(\Omega^{(e)})} \mathbf{B}^T \mathbf{\hat{\sigma}} dV \approx \sum_{i=1}^{n_{gp}} w_i J_i \mathbf{B}^T_i \mathbf{\hat{\sigma}}_i \]  

(2.73)
Box 1: The incremental non-linear finite element scheme - implicit solution.

1. Assemble the global external force vector, $\bar{f}^{ext}$
2. Initialize increment counter $i = 1$
3. Set load factor , $\lambda_i$
4. Solve the non-linear equilibrium equation
   \[ r(u_{n+1}) = f^{int}(u_{n+1}) - \lambda_i \bar{f}^{ext} = 0 \]
5. Update increment counter $i = i + 1$
6. Check if prescribed number of increments has been achieved

where $w_i$ and $J_i$ are, respectively, the Gaussian weight and the Jacobian at the $i^{th}$ integration point. A similar procedure is carried out for the external force vector.

**Newton-Raphson method**

As stressed out before, the equilibrium equation (2.68) is generally non-linear and demands an appropriate solution method. We will adopt herein the Newton-Raphson method, which is particularly attractive due to its quadratic rates of convergence. Following standard procedures of the method and particularising for the case of the finite element framework presented in this chapter, the displacements are updated according to:

\[ u_{n+1}^{k+1} = u_{n+1}^k - \left( \frac{\partial r}{\partial u_{n+1}} \bigg|_{u_{n+1}^k} \right)^{-1} r(u_{n+1}^k) \]  (2.74)

Equation (2.74) can be more conveniently written as

\[ K_T \delta u = -r(u_{n+1}^k), \]  (2.75)

where

\[ u = u_{n+1}^{k+1} - u_{n+1}^k, \]  (2.76)

and $K_T$ is called global tangent stiffness matrix, given by

\[ K_T = \frac{\partial r}{\partial u_{n+1}} \bigg|_{u_{n+1}^k}. \]  (2.77)

The correct derivation of the tangent stiffness is crucial to guarantee the quadratic rates of convergence of the Newton-Raphson method. In the case of finite strains
within a spatial description, the expression for Equation (2.77) arises quite naturally from the linearisation of the equilibrium equation in its weak form. Recalling that the internal force vector is integrated using a Gaussian quadrature (Equation 2.73), the element stiffness matrix is then given by:

\[
K^{(e)}_T = \sum_{i=1}^{nqp} w_i J_i \mathbf{B}_i^T \mathbf{\tilde{a}}_i \mathbf{G}_i, \tag{2.78}
\]

where \( \mathbf{a}_i \) is the spatial tangent modulus whose components are given by

\[
a_{ijkl} = \frac{1}{J} \frac{\partial \tau_{ij}}{\partial F_{km}} F_{lm} \sigma_{il} \delta_{jk}. \tag{2.79}
\]

For convenience, the full Newton-Raphson procedure associated with the present finite element framework at finite strains is summarised in Box 2.

Box 2: Newton-Raphson scheme for the solution of the incremental non-linear finite element equilibrium equation implicit solution.
1. Set \( k = 1 \), initial guess and residual function array
\[
\mathbf{u}^{k+1}_n = \mathbf{u}_n; \quad \mathbf{r}^k = \mathbf{f}^{\text{int}}(\mathbf{u}_n) - \lambda_{n+1} \overline{\mathbf{f}}^{\text{ext}}
\]

2. Compute the consistent spatial tangent moduli
\[
a_{ijkl} = \frac{1}{J} \frac{\partial r_{ij}}{\partial F_{km}} F_{lm} - \sigma^{il} \delta_{jk}.
\]

3. Assemble element tangent stiffness matrices
\[
K^{(e)}_T = \sum_{i=1}^{ngp} w_i J_i \mathbf{B}_i^T \hat{\mathbf{a}}_i \mathbf{G}_i,
\]

4. Assemble global stiffness and solve for \( \delta \mathbf{u}^{k+1} \)
\[
K_T \delta \mathbf{u}^{k+1} = -\mathbf{r}^k
\]

5. Update displacements
\[
\mathbf{u}^{k+1}_n = \mathbf{u}^k_n + \delta \mathbf{u}^{k+1}
\]

6. Update the deformation gradient
\[
F^{k+1}_{n+1} = (I + \nabla_x \mathbf{u}^{k+1}_n)^{-1}
\]

7. Update stresses and internal variables
\[
\sigma^{k+1}_n = \hat{\sigma}(F^{k+1}_{n+1}; \alpha_n); \quad \alpha^{k+1}_n = \hat{\alpha}(F^{k+1}_{n+1}; \alpha_n)
\]

8. Compute element internal force
\[
f^{\text{int}}_{(e)} = \sum_{i=1}^{ngp} w_i J_i \mathbf{B}_i^T \hat{\sigma}^{k+1}_{n+1}
\]

9. Assemble the global internal force array and re-compute the residual function
\[
\mathbf{r}^{k+1} = \mathbf{f}^{\text{int}} - \lambda_{n+1} \overline{\mathbf{f}}^{\text{ext}}
\]

10. Check convergence IF \( \| \mathbf{r}^{k+1} \| < TOL \) EXIT

11. Set \( k = k + 1 \) and go to (2).
Chapter 3

BPA based model

3.1 Introduction

During the last decades, several researchers have worked in the field of constitutive modeling of polymers and used the finite element method for analysing problems with polymeric materials. Academic community has followed different approaches for the modeling of mechanical behavior of polymers. For a review on the topic the reader is referred to Mackerle (1997), Mackerle (2003).

There is a quite vast area of applications for polymers including electronic, automotive and medical industries. It is worth emphasizing the using polymeric based materials in different industries is being increased due to interesting mechanical, thermal and processing properties.

This chapter introduces a finite strain elasto-viscoplastic constitutive model. The flow potential of the model is based on the Argon theory taken from BPA model (Boyce et al., 1988). The model is shown to be able to describe to typical deformation behavior of thermoplastics namely, initial elastic, yield, post yield softening and final hardening.

Next section describes the finite strain elasto-viscoplastic constitutive model.

3.2 Formulation

In this section, a finite strain multiplicative model for polymeric materials is described. In order to develop a finite strain constitutive model, different issues have to be addressed. First of, the kinematics of finite strain should be explained. Dissipation potential is probably the most important part of the constitutive model that has to
be characterized.
In the following section we describe the multiplicative kinematic. Then a logarithmic strain measure will be introduced. Free energy potential, dissipation potential and additive decomposition of the stress are addressed.

### 3.2.1 Multiplicative kinematics

Multiplicative decomposition of the deformation gradient into an elastic and a plastic contribution is adopted for this study. In fact, this elastic plastic decomposition of the total deformation gradient is widely used, due its suitable features, by different authors for developing constitutive models not only for polymers but also for other class of materials such as metals, etc. According to the multiplicative kinematics, the total deformation gradient, \( F \), is composed by the elastic deformation gradient, \( F^e \), and plastic deformation gradient, \( F^p \). Details regarding this multiplicative kinematics could be found in De Souza Neto et al. (2008).

\[
F = F^e F^p
\]

(3.1)

In order to understand the multiplicative kinematics better, Figure (3.1) explains this decomposition.

![Figure 3.1: Elastic-Plastic decomposition of the total deformation gradient](Reproduced from De Souza Neto et al. (2008))

It can be said that using this multiplicative kinematics, relation (3.1), implies the
existence of an intermediate configuration which is unstressed and is obtained by elastic unloading from the final deformed configuration.

Both elastic and plastic deformation gradients, could be polar decomposed as provided by relations (3.2) and (3.3).

\[
F^e = R^e U^e = V^e R^e, \quad (3.2)
\]

\[
F^p = R^p U^p = V^p R^p, \quad (3.3)
\]
polar decomposition of the deformation gradient is explained graphically is Figure (3.2).

Figure 3.2: Polar decomposition of the deformation gradient-Reproduced from De Souza Neto et al. (2008)

The components of the polar decomposition, \(R^e, U^e\) and \(V^e\) are the elastic rotation tensor, elastic right stretch tensor and elastic left stretch tensor, respectively. The terms in relation (3.3) are the corresponding plastic terms. The definition of the velocity gradient is provided below.

\[
\dot{L} = \dot{F} F^{-1}. \quad (3.4)
\]

Using multiplicative kinematics, relation (3.1), in velocity gradient, equation (3.4), gives:

\[
\dot{L} = L^e + F^e L^p (F^e)^{-1}, \quad (3.5)
\]
where, $L^e$ is the elastic velocity gradient and $L^p$ is the plastic deformation gradient defined by following relations.

$$L^e \equiv \dot{\mathbf{F}}^e (\mathbf{F}^e)^{-1},\quad (3.6)$$

$$L^p \equiv \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1}.\quad (3.7)$$

Symmetric and skew part of the plastic velocity gradient are given below:

$$D^p \equiv \text{sym} (L^p) = \frac{1}{2} \left[ L^p + (L^p)^T \right],\quad (3.8)$$

$$W^p \equiv \text{skew} (L^p) = \frac{1}{2} \left[ L^p - (L^p)^T \right],\quad (3.9)$$

where, the superscript $T$ stands for transpose. $D^p$ is called plastic stretching tensor or the rate of plastic deformation and $W^p$ is called plastic spin tensor. It should be mentioned that the plastic spin tensor is assumed to be zero.

$$W^p = 0 \quad (3.10)$$

Boyce et al. (1989) and Timmermans (1998) explained that in case of polymeric materials, having different plastic spin tensors is not of great effect on the overall deformation behaviour. Consequently, assuming plastic spin tensor null, does not considerably changes the stress-strain curve predicted by the model.

### 3.2.2 Strain measure

In this chapter, in order to measure the elastic deformations, natural (logarithmic) spatial (Eulerian) strain is chosen. The reason for choosing the strain measure is because of its physical meaning. Moreover, adopting logarithmic strain measure helps to simplify the stress integration algorithm in a sense that the small strain elastic predictor/return mapping algorithm is easily extended to finite strains.

The definition of logarithmic elastic strain tensor is given in:

$$\varepsilon^e \equiv \ln \mathbf{V}^e = \frac{1}{2} \ln \mathbf{B}^e\quad (3.11)$$

In relation (3.11), the logarithm operator, $\ln(\bullet)$, is tensorial logarithm of $\bullet$. Left elastic Cauchy-Green deformation tensor is defined by relation (3.12)

$$\mathbf{B}^e \equiv \mathbf{F}^e [\mathbf{F}^e]^T = [\mathbf{V}^e]^2.\quad (3.12)$$
3.2.3 Flow potential

The dissipation potential and flow rule of the model are defined using the Argon theory. The plastic stretching tensor at the current configuration is given by:

\[ d^p = \dot{\gamma}^p \frac{\partial \Psi}{\partial \sigma} = \dot{\gamma}^p N, \tag{3.13} \]

where, \( \Psi \) is a dissipation potential, \( N \) is a flow vector and \( d^p \) is spatial plastic stretching tensor:

\[ d^p \equiv R^e D^p R^{eT}. \tag{3.14} \]

Different terms in relation (3.14) could be explained and interpreted as follows:

- \( D^p \) is plastic stretching tensor in the relaxed configuration.
- \( d^p \) is plastic stretching tensor in the current configuration (rotated from intermediate configuration using elastic rotation).

As stated above, the flow vector \( N \) is the derivative of dissipation potential in order to stress. Hence, the dissipation potential should be defined in order to obtain the flow vector. The dissipation potential is assumed to be:

\[ \Psi = \sqrt{\frac{1}{2}} s : s. \tag{3.15} \]

As a result, the flow vector is obtained:

\[ N = \frac{\partial \Psi}{\partial \sigma} = \sqrt{\frac{1}{2}} \frac{s}{||s||}, \tag{3.16} \]

where, \( ||s|| \) is the norm of \( s \) defined by:

\[ ||s|| = \sqrt{s : s}. \tag{3.17} \]

Combining relations (3.13) and (3.16), the multi-dimensional plastic flow rule of the model is obtained as:

\[ d^p = \dot{\gamma}^p \sqrt{\frac{1}{2}} \frac{s}{||s||}. \tag{3.18} \]

Plastic shear strain rate, \( \dot{\gamma}^p \), is given by:

\[ \dot{\gamma}^p = \dot{\gamma}_0 \exp \left( -\frac{\Delta G^*}{kT} \right), \tag{3.19} \]

where, \( \dot{\gamma}_0 \) is pre-exponential shear strain rate factor (one of the material properties); \( k \) is Boltzmanns constant; \( T \) is the absolute temperature and \( \Delta G^* \) is the free energy change. The free energy change is given by:

\[ \Delta G^* = \frac{3\pi \mu \omega^2 \alpha^3}{16(1 - \nu)} \left[ 1 - \left( \frac{\tau}{0.07 \mu} \right)^{(5/6)} \right], \tag{3.20} \]
where, $\mu$ is shear modulus; $\nu$ is poisson's ratio; $\omega$ is the net angle of rotation of the molecular segment between the initial configuration and the activated configuration and $\alpha$ is the mean molecular radius. Relation (3.19) can be rewritten as follows:

$$\dot{\gamma}^p = \dot{\gamma}_0 \exp \left[ -\frac{A\tilde{s}}{T} \left( 1 - \left( \frac{\tau}{\tilde{s}} \right)^{(b/6)} \right) \right],$$  \hspace{1cm} (3.21)

where, $\tau$ is the shear stress. The parameter $\tilde{s}$ is given by:

$$\tilde{s} = s + \alpha p, \hspace{1cm} (3.22)$$

where, $p$ is hydrostatic pressure. The evolution of $s$ is characterized by:

$$\dot{s} = h \left( 1 - \frac{s}{s_{ss}} \right) \dot{\gamma}^p, \hspace{1cm} (3.23)$$

$$s = s_0 + \alpha p \hspace{1cm} (3.24)$$

$A$ and $s_0$ are defined by relations (3.25) and (3.26), respectively.

$$A \equiv \frac{39\pi\omega^2\alpha^3}{16K}, \hspace{1cm} (3.25)$$

$$s_0 \equiv \frac{0.077\mu}{1 - \nu}. \hspace{1cm} (3.26)$$

### 3.2.4 Stress decomposition

The total stress, $\sigma^{total}$, of the model, is additively composed of driving stress and hardening stress:

$$\sigma^{total} = \sigma^{driving} + \sigma^{hardening}. \hspace{1cm} (3.27)$$

In this study, the hardening stress is not taken into account. Since the main objective of this thesis is to use numerical methods, Finite Element Method and Newton-Raphson method, to solve the nonlinear system of equations of equilibrium, the total stress is assumed to be the driving component of the stress.

### 3.3 Conclusions

In this chapter a finite strain elasto-viscoplastic constitutive model was introduced. The kinematic and material contribution of the constitutive model were introduced. The description of the flow potential, which is in fact the core of the model, was introduced by Boyce et al. (1988) and the model is known as BPA model.
Chapter 4

The integration algorithm of the model

4.1 Introduction

This chapter deals with the integration algorithm of the model introduced in chapter (3). Stress integration algorithm and consistent tangent operator are explained. The numerical implementation of stress integration algorithm and tangent operator is demonstrated. (Ortiz et al. (1983); Zienkiewicz and Taylor (1991); Owen and Hinton (1980); De Souza Neto et al. (2008); (Simo and Hughes, 1998); Simo et al. (1998)) studied numerical solution of constitutive models within finite element approach which basically is solution of a set of evolutionary equations in an iterative fashion.

The solution pursued in this study has a strain driven structure and is performed at each Gauss point of the finite element mesh. Stress and internal variables are updated according to the the level of current strain and the values of the internal variables in the previous increment.

In order to have the solution of the global boundary value problem, using Newton-Raphson method, efficiently converged, the consistent linearization of the time discretized constitutive equations is very important.

Using operator split algorithms are nowadays standard procedure for numerical integration of elasto-plastic and elasto-viscoplastic constitutive equations (Criesfield (1997); Simo and Hughes (1998)). In order to implement the constitutive model into a finite element code, it is required to derive the state update equations and also consistent tangent operator. The state update procedure is derived using operator split algorithm and as a result an elastic predictor/return mapping algorithm is obtained for the state update procedure.
4.2 State update

It is worth emphasizing that state update and consistent tangent are derived on the small strain format of the constitutive equations. Then they are extended to finite strain as explained (De Souza Neto et al., 2008).

4.2 State update

In this section, the constitutive equations of the model introduced in chapter (3) are time discretized and operator split algorithm is applied to the equations in order to derive the elastic predictor/return mapping algorithm of the state update procedure. Initially, the total strain at the beginning of state update is assumed elastic (this stage is called elastic predictor) and then using the return mapping equations (derived from the flow potential and other constitutive equations), the inelastic contribution of the total strain would be determined through an iterative procedure (this stage is called plastic corrector or return mapping).

4.2.1 Return mapping

In order to update the deformation gradient and obtain the deformation gradient at time step \( t_{n+1} \), we use:

\[
F_{n+1} = F_\Delta F_n. \tag{4.1}
\]

where, \( F_{n+1} \) is the deformation gradient at \( t_{n+1} \), \( F_n \) is the deformation gradient at \( t_n \) and \( F_\Delta \) is the incremental deformation gradient. Considering incremental displacement known, the incremental deformation gradient is obtained by:

\[
F_\Delta = I + \nabla_n(\Delta u), \tag{4.2}
\]

where, \( \nabla_n(\Delta u) \) is the gradient of the incremental displacement.

We need to obtain the elastic trial state so that we will then apply return mapping procedure in order to determine which part of the strain has been elastic and which part has been plastic strain. As we know the total elastic strain at \( t_n \) which is \( \varepsilon_n^e \), the elastic left Cauchy-Green deformation tensor is obtained by:

\[
B_n^e = \exp[2 \varepsilon_n^e]. \tag{4.3}
\]

The elastic trial left Cauchy-Green deformation tensor at \( t_{n+1} \) is given by:

\[
B_{n+1}^{e \, trial} = F_\Delta B_n^e (F_\Delta)^T. \tag{4.4}
\]
Having elastic trial left Cauchy-Green deformation tensor computed, the driving parameter of the study which is the elastic trial strain at \( t_{n+1} \) i.e. \( \varepsilon_{n+1}^{\text{trial}} \) is given by:

\[
\varepsilon_{n+1}^{\text{trial}} = \ln [V_{n+1}^{\text{trial}}] = \frac{1}{2} \ln [B_{n+1}^{\text{trial}}].
\]  

(4.5)

It is worth noting that so far, everything is independent of the material models i.e. everything is done at the kinematic level and for whatever constitutive model could be used. At this stage, when we have the elastic trial strain determined, the stresses and state variables should be updated using the constitutive relations.

In order to derive the integration algorithm of the model, the small strain counterpart of relation (3.18) is used:

\[
\dot{\gamma}^p = \dot{\gamma}^0 \sqrt{\frac{1}{2} \frac{s}{||s||}},
\]  

(4.6)

where, \( s \) is the deviatoric part of the Kirchhoff stress.

\[
s = I_d : \tau,
\]  

(4.7)

and \( ||s|| \) is the norm of the deviatoric stress.

\[
||s|| = \sqrt{s : s}.
\]  

(4.8)

Integration of relation (4.6) over the time step \([t_n, t_{n+1}]\) gives:

\[
\varepsilon_{n+1}^p - \varepsilon_n^p = \dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2} \frac{\Delta t}{||s_{n+1}||}} s_{n+1}
\]  

(4.9)

The time discretized form of relation (3.21) is given by:

\[
\dot{\gamma}_{n+1}^p = \dot{\gamma}_0 \exp \left[ -A \tilde{s}_{n+1} \left( 1 - \left( \frac{\tau}{s_{n+1}} \right)^{(5/6)} \right) \right],
\]  

(4.10)

where,

\[
\tilde{s}_{n+1} = s_{n+1} + \alpha p_{n+1}
\]  

(4.11)

Integrating relation (3.23) over time step \([t_n, t_{n+1}]\) gives relation (4.12):

\[
s_{n+1} - s_n - h \left( 1 - \frac{s_{n+1}}{s_{ss}} \right) \dot{\gamma}_{n+1}^p \Delta t = 0
\]  

(4.12)
From relation (4.9), the following system of four non-linear equations are obtained:

\[
\begin{align*}
\Delta \varepsilon_{n+1}^P(1) &= \dot{\gamma}_{n+1} P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(1) \\
\Delta \varepsilon_{n+1}^P(2) &= \dot{\gamma}_{n+1} P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(2) \\
\Delta \varepsilon_{n+1}^P(3) &= \dot{\gamma}_{n+1} P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(3) \\
\Delta \varepsilon_{n+1}^P(4) &= \dot{\gamma}_{n+1} P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(4)
\end{align*}
\]

(4.13)

Considering relations (4.10)-(4.12), and the system of equations (4.13), the following system of six algebraic equations are obtained, in the two dimensional space, for the finite element implementation of the model.

\[
\begin{align*}
R_1 &:= \Delta \varepsilon_{n+1}^P(1) - \dot{\gamma}_{n+1} P P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(1) = 0 \\
R_2 &:= \Delta \varepsilon_{n+1}^P(2) - \dot{\gamma}_{n+1} P P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(2) = 0 \\
R_3 &:= \Delta \varepsilon_{n+1}^P(3) - \dot{\gamma}_{n+1} P P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(3) = 0 \\
R_4 &:= \Delta \varepsilon_{n+1}^P(4) - \dot{\gamma}_{n+1} P P \sqrt{\frac{1}{2} \frac{\Delta t}{|s_n+1|}} s_{n+1}(4) = 0 \\
R_5 &:= \dot{\gamma}_{n+1} P - \dot{\gamma}_0 \exp \left[ -\frac{A\tau_{n+1}}{\tau} \left( 1 - \left( \frac{s_{n+1}}{s_{n+1}} \right)^{5/6} \right) \right] = 0 \\
R_6 &:= s_{n+1} - s_n - \dot{h} \left( 1 - \frac{s_{n+1}}{s_{n+1}} \right) \dot{\gamma}_{n+1} P \Delta t = 0
\end{align*}
\]

(4.14)

The unknowns of the system of equations (4.14) are $\Delta \varepsilon_{n+1}^P(1)$, $\Delta \varepsilon_{n+1}^P(2)$, $\Delta \varepsilon_{n+1}^P(3)$, $\Delta \varepsilon_{n+1}^P(4)$, $\dot{\gamma}_{n+1}$ and $s_{n+1}$. The system of equation will be solved using the well-known iterative Newton-Raphson method. The unknowns are called $u_1$, $u_2$, $u_3$, $u_4$, $u_5$ and $u_6$, respectively. In order to solve the system of equations using the Newton-Raphson method in an iterative fashion, the derivatives of all equations in order to all unknowns should be calculated:

\[
\begin{bmatrix}
\frac{\partial R_1}{\partial u_1} & \frac{\partial R_1}{\partial u_2} & \frac{\partial R_1}{\partial u_3} & \cdots & \frac{\partial R_1}{\partial u_6} \\
\frac{\partial R_2}{\partial u_1} & \frac{\partial R_2}{\partial u_2} & \frac{\partial R_2}{\partial u_3} & \cdots & \frac{\partial R_2}{\partial u_6} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{\partial R_6}{\partial u_1} & \frac{\partial R_6}{\partial u_2} & \frac{\partial R_6}{\partial u_3} & \cdots & \frac{\partial R_6}{\partial u_6}
\end{bmatrix}
\begin{bmatrix}
\delta u_1 \\
\delta u_2 \\
\vdots \\
\delta u_6
\end{bmatrix}
= - \begin{bmatrix}
R_1 \\
R_2 \\
\vdots \\
R_6
\end{bmatrix}
\]

(4.15)
Where, superscripts \( k-1 \) and \( k \) stand for two consecutive Newton-Raphson iterations. The required derivatives in relation (4.15) are provided below.

**Derivatives of the first residual equation**

Derivative of the first residual equation in order to first unknown:

\[
\frac{\partial R_1}{\partial u_1} = 1 - \dot{\gamma}^p_{n+1} \sqrt{\frac{1}{2} \Delta t} \, C_1, \quad (4.16)
\]

where,

\[
C_1 = \frac{||s_{n+1}||C_2 - s_{n+1}(1)C_3}{(||s_{n+1}||)^2}, \quad (4.17)
\]

where, \( C_2 \) and \( C_3 \) are given by:

\[
C_2 = -2G, \quad C_3 = \frac{-2Gs_{n+1}(1)}{||s_{n+1}||}. \quad (4.18)
\]

Derivative of the first residual equation in order to second unknown:

\[
\frac{\partial R_1}{\partial u_2} = -\dot{\gamma}^p_{n+1} \sqrt{\frac{1}{2} \Delta t} \, C_4, \quad (4.19)
\]

where, we have:

\[
C_4 = -\frac{s_{n+1}(1)C_5}{(||s_{n+1}||)^2}, \quad C_5 = -2Gs_{n+1}(2) \frac{||s_{n+1}||}{||s_{n+1}||}. \quad (4.20)
\]

Derivative of the first residual equation in order to third unknown:

\[
\frac{\partial R_1}{\partial u_3} = -\dot{\gamma}^p_{n+1} \sqrt{\frac{1}{2} \Delta t} \, C_6, \quad (4.21)
\]

where,

\[
C_6 = -\frac{s_{n+1}(1)C_7}{(||s_{n+1}||)^2}, \quad C_7 = -4Gs_{n+1}(3) \frac{||s_{n+1}||}{||s_{n+1}||}. \quad (4.22)
\]

Derivative of the first residual equation in order to fourth unknown:

\[
\frac{\partial R_1}{\partial u_4} = -\dot{\gamma}^p_{n+1} \sqrt{\frac{1}{2} \Delta t} \, C_8, \quad (4.23)
\]

where,

\[
C_8 = -\frac{s_{n+1}(1)C_9}{(||s_{n+1}||)^2}, \quad C_9 = -2Gs_{n+1}(4) \frac{||s_{n+1}||}{||s_{n+1}||}. \quad (4.24)
\]

Derivative of the first residual equation in order to fifth unknown:

\[
\frac{\partial R_1}{\partial u_5} = -\sqrt{\frac{1}{2} \Delta t} \frac{s_{n+1}(1)}{||s_{n+1}||}. \quad (4.25)
\]
4.2 State update

Derivative of the first residual equation in order to sixth unknown:

\[ \frac{\partial R_1}{\partial u_6} = 0. \]  (4.26)

Derivatives of the second residual equation

Derivative of the second residual equation in order to first unknown:

\[ \frac{\partial R_2}{\partial u_1} = -\dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2}\Delta t} C_{10}, \]  (4.27)

where,

\[ C_{10} = -s_{n+1}^{(2)} C_3 / (||s_{n+1}||)^2. \]  (4.28)

Derivative of the second residual equation in order to second unknown:

\[ \frac{\partial R_2}{\partial u_2} = 1 - \dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2}\Delta t} C_{11}, \]  (4.29)

where,

\[ C_{11} = ||s_{n+1}|| C_{12} - s_{n+1}^{(2)} C_5 / (||s_{n+1}||)^2, \]  (4.30)

where, \( C_{12} \) and is given by:

\[ C_{12} = -2G. \]  (4.31)

Derivative of the second residual equation in order to third unknown:

\[ \frac{\partial R_2}{\partial u_3} = -\dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2}\Delta t} C_{13}, \]  (4.32)

where,

\[ C_{13} = -s_{n+1}^{(2)} C_7 / (||s_{n+1}||)^2. \]  (4.33)

Derivative of the second residual equation in order to fourth unknown:

\[ \frac{\partial R_2}{\partial u_4} = -\dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2}\Delta t} C_{14}, \]  (4.34)

where,

\[ C_{14} = -s_{n+1}^{(2)} C_9 / (||s_{n+1}||)^2. \]  (4.35)

Derivative of the second residual equation in order to fifth unknown:

\[ \frac{\partial R_2}{\partial u_5} = -\sqrt{\frac{1}{2}\Delta t} s_{n+1}^{(2)} / ||s_{n+1}||. \]  (4.36)
4.2 State update

Derivative of the second residual equation in order to sixth unknown:

\[
\frac{\partial R_2}{\partial u_6} = 0.
\]  \hfill (4.37)

**Derivatives of the third residual equation**

Derivative of the third residual equation in order to first unknown:

\[
\frac{\partial R_3}{\partial u_1} = -\gamma_{n+1}^p \sqrt{\frac{1}{2} \Delta t} C_{15},
\]  \hfill (4.38)

where,

\[
C_{15} = -\frac{s_{n+1}(3) C_3}{(||s_{n+1}||)^2}.
\]  \hfill (4.39)

Derivative of the third residual equation in order to second unknown:

\[
\frac{\partial R_3}{\partial u_2} = -\gamma_{n+1}^p \sqrt{\frac{1}{2} \Delta t} C_{16},
\]  \hfill (4.40)

where,

\[
C_{16} = -\frac{s_{n+1}(3) C_5}{(||s_{n+1}||)^2}.
\]  \hfill (4.41)

Derivative of the third residual equation in order to third unknown:

\[
\frac{\partial R_3}{\partial u_3} = 1 - \gamma_{n+1}^p \sqrt{\frac{1}{2} \Delta t} C_{17},
\]  \hfill (4.42)

where,

\[
C_{17} = \frac{||s_{n+1}|| C_{18} - s_{n+1}(3) C_7}{(||s_{n+1}||)^2},
\]  \hfill (4.43)

where, \( C_{18} \) and is given by:

\[
C_{18} = -2G.
\]  \hfill (4.44)

Derivative of the third residual equation in order to fourth unknown:

\[
\frac{\partial R_3}{\partial u_4} = -\gamma_{n+1}^p \sqrt{\frac{1}{2} \Delta t} \left( -\frac{s_{n+1}(3) C_9}{(||s_{n+1}||)^2} \right).
\]  \hfill (4.45)

Derivative of the third residual equation in order to fifth unknown:

\[
\frac{\partial R_3}{\partial u_5} = -\sqrt{\frac{1}{2} \Delta t} \frac{s_{n+1}(3)}{||s_{n+1}||}.
\]  \hfill (4.46)

Derivative of the third residual equation in order to sixth unknown:

\[
\frac{\partial R_3}{\partial u_6} = 0.
\]  \hfill (4.47)
Derivatives of the fourth residual equation

Derivative of the fourth residual equation in order to first unknown:

$$\frac{\partial R_4}{\partial u_1} = -\dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2} \Delta t} C_{19}, \quad (4.48)$$

where,

$$C_{19} = -\frac{s_{n+1}(4)C_3}{(||s_{n+1}||)^2}. \quad (4.49)$$

Derivative of the fourth residual equation in order to second unknown:

$$\frac{\partial R_4}{\partial u_2} = -\dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2} \Delta t} C_{20}, \quad (4.50)$$

where,

$$C_{20} = -\frac{s_{n+1}(4)C_5}{(||s_{n+1}||)^2}. \quad (4.51)$$

Derivative of the fourth residual equation in order to third unknown:

$$\frac{\partial R_4}{\partial u_3} = -\dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2} \Delta t} C_{21}, \quad (4.52)$$

where,

$$C_{21} = -\frac{s_{n+1}(4)C_7}{(||s_{n+1}||)^2}. \quad (4.53)$$

Derivative of the fourth residual equation in order to fourth unknown:

$$\frac{\partial R_4}{\partial u_4} = 1 - \dot{\gamma}_{n+1}^p \sqrt{\frac{1}{2} \Delta t} C_{22}, \quad (4.54)$$

where,

$$C_{22} = ||s_{n+1}||C_{23} - s_{n+1}(4)C_9 \quad (||s_{n+1}||)^2. \quad (4.55)$$

where, $C_{18}$ and is given by:

$$C_{23} = -2G \quad (4.56)$$

Derivative of the third residual equation in order to fifth unknown:

$$\frac{\partial R_4}{\partial u_5} = -\sqrt{\frac{1}{2} \Delta t} \frac{s_{n+1}(4)}{||s_{n+1}||}. \quad (4.57)$$

Derivative of the fourth residual equation in order to sixth unknown:

$$\frac{\partial R_4}{\partial u_6} = 0. \quad (4.58)$$
Derivatives of the fifth residual equation

Derivative of the fifth residual equation in order to first unknown:

\[
\frac{\partial R_5}{\partial u_1} = -\dot{\gamma}_0 \exp(C_{24}) C_{25}, \tag{4.59}
\]

where,

\[
C_{24} = -\frac{A\tilde{s}_{n+1}}{T} \left(1 - \left(\frac{\tau_{n+1}}{\tilde{s}_{n+1}}\right)^{(5/6)}\right), \tag{4.60}
\]

and

\[
C_{25} = \left(\frac{5}{6}\right) \frac{A\tilde{s}_{n+1}}{T} \left(\frac{\tau_{n+1}}{\tilde{s}_{n+1}}\right)^{(-1/6)} C_{26}, \tag{4.61}
\]

where, \(C_{26}\) is given by:

\[
C_{26} = \frac{1}{\tilde{s}_{n+1}} C_{27}, \quad C_{27} = \frac{C_3}{\sqrt{2}}. \tag{4.62}
\]

Derivative of the fifth residual equation in order to second unknown:

\[
\frac{\partial R_5}{\partial u_2} = -\dot{\gamma}_0 \exp(C_{24}) C_{28}, \tag{4.63}
\]

where,

\[
C_{28} = \left(\frac{5}{6}\right) \frac{A\tilde{s}_{n+1}}{T} \left(\frac{\tau_{n+1}}{\tilde{s}_{n+1}}\right)^{(-1/6)} C_{29}, \tag{4.64}
\]

where, \(C_{29}\) is given by:

\[
C_{26} = \frac{1}{\tilde{s}_{n+1}} C_{30}, \quad C_{30} = \frac{C_5}{\sqrt{2}}. \tag{4.65}
\]

Derivative of the fifth residual equation in order to third unknown:

\[
\frac{\partial R_5}{\partial u_3} = -\dot{\gamma}_0 \exp(C_{24}) C_{31}, \tag{4.66}
\]

where,

\[
C_{31} = \left(\frac{5}{6}\right) \frac{A\tilde{s}_{n+1}}{T} \left(\frac{\tau_{n+1}}{\tilde{s}_{n+1}}\right)^{(-1/6)} C_{32}, \tag{4.67}
\]

where, \(C_{32}\) is given by:

\[
C_{32} = \frac{1}{\tilde{s}_{n+1}} C_{33}, \quad C_{33} = \frac{C_7}{\sqrt{2}}. \tag{4.68}
\]

Derivative of the fifth residual equation in order to fourth unknown:

\[
\frac{\partial R_5}{\partial u_3} = -\dot{\gamma}_0 \exp(C_{24}) \left(\frac{5}{6}\right) \frac{A\tilde{s}_{n+1}}{T} \left(\frac{\tau_{n+1}}{\tilde{s}_{n+1}}\right)^{(-1/6)} C_{34}, \tag{4.69}
\]
where, $C_{34}$ is given by:

$$C_{34} = \frac{1}{\tilde{s}_{n+1}} C_{35} \quad , \quad C_{35} = \frac{C_0}{\sqrt{2}}.$$  (4.70)

Derivative of the fifth residual equation in order to fifth unknown:

$$\frac{\partial R_5}{\partial u_5} = 1 - \dot{\gamma}_0 \exp (C_{24}) C_{36},$$  (4.71)

where, $C_{36}$ is equal to:

$$C_{36} = \left( 1 - \left( \frac{\tau_{n+1}}{S_{n+1}} \right)^{(5/6)} \right) C_{37} - \left( A \tilde{s}_{n+1} T \right) C_{38},$$  (4.72)

where, $C_{37}$ and $C_{38}$ are given by:

$$C_{37} = -\frac{A}{T} C_{39},$$  (4.73)

$$C_{38} = \frac{5}{6} \left( \frac{\tilde{s}_{n+1}}{\tau_{n+1}} \right)^{(1/6)} \frac{\tau_{n+1}}{(s_{n+1})^2} C_{39},$$  (4.74)

where, $C_{39}$, is given by the following relation:

$$C_{39} = \frac{s_{ss} h \Delta t \left( s_{ss} + h \gamma_{n+1}^p \Delta t \right) - h \Delta t \left( s_{ss} \left( s_n + h \gamma_{n+1}^p \Delta t \right) \right)}{(s_{ss} + h \gamma_{n+1}^p \Delta t)^2}.$$  (4.75)

Derivative of the fifth residual equation in order to sixth unknown:

$$\frac{\partial R_5}{\partial u_6} = -\dot{\gamma}_0 \exp (C_{24}) C_{40},$$  (4.76)

where, $C_{40}$ is given by:

$$C_{40} = -\frac{A}{T} \left( 1 - \left( \frac{\tau_{n+1}}{S_{n+1}} \right)^{(5/6)} \right) + \left( \frac{5}{6} \right) \frac{A \tilde{s}_{n+1}}{T} \left( \frac{\tau_{n+1}}{S_{n+1}} \right)^{(1/6)} C_{41},$$  (4.77)

where,

$$C_{41} = -\frac{\tau_{n+1}}{(s_{n+1})^2}.$$  (4.78)

**Derivatives of the sixth residual equation**

Derivatives of the sixth residual equation in order to first four unknowns are equal to zero.

$$\frac{\partial R_6}{\partial u_1} = \frac{\partial R_6}{\partial u_2} = \frac{\partial R_6}{\partial u_3} = \frac{\partial R_6}{\partial u_4} = 0.$$  (4.79)
4.3 Consistent tangent operator

Derivative of the sixth residual equation in order to fifth unknown:

\[ \frac{\partial R_6}{\partial u_5} = -h\Delta t \left( 1 - \frac{s_{n+1}}{s_{ss}} \right). \]  \hfill (4.80)

Derivative of the sixth residual equation in order to sixth unknown:

\[ \frac{\partial R_6}{\partial u_6} = 1 + \frac{h\gamma p}{s_{ss}} \Delta t. \]  \hfill (4.81)

Having all the derivatives computed, it is possible to introduce the relation (4.16)-(4.81), into the system of equations (4.15) and solve it using Newton-Raphson method in an iterative manner. After solving the system of equations, we have:

\[ u_1^k = \Delta \varepsilon_{n+1}^{P,k}(1) = \Delta \varepsilon_{n+1}^{P,k-1}(1) + (\delta u_1)^k, \]  \hfill (4.82)

\[ u_2^k = \Delta \varepsilon_{n+1}^{P,k}(2) = \Delta \varepsilon_{n+1}^{P,k-1}(2) + (\delta u_2)^k, \]  \hfill (4.83)

\[ u_3^k = \Delta \varepsilon_{n+1}^{P,k}(3) = \Delta \varepsilon_{n+1}^{P,k-1}(3) + (\delta u_3)^k, \]  \hfill (4.84)

\[ u_4^k = \Delta \varepsilon_{n+1}^{P,k}(4) = \Delta \varepsilon_{n+1}^{P,k-1}(4) + (\delta u_4)^k, \]  \hfill (4.85)

\[ u_5^k = \dot{\gamma}_{n+1}^{p,k} = \dot{\gamma}_{n+1}^{p,k-1} + (\delta u_5)^k, \]  \hfill (4.86)

\[ u_6^k = s_{n+1}^k = s_{n+1}^{k-1} + (\delta u_6)^k. \]  \hfill (4.87)

4.3 Consistent tangent operator

For the sake of completing the finite element implementation of the model, it is required to derive the tangent operator due to the fact that the tangent operator is the only material related term in the global tangent stiffness matrix. De Souza Neto et al. (2008) introduced the spatial global tangent stiffness by:

\[ a_{ijkl} = \frac{1}{J} \left[ D : \mathbf{L} : \mathbf{B} \right]_{ijkl} - \sigma_{ij} \delta_{jk}, \]  \hfill (4.88)

where, \( \delta \) is the Kronecker delta, \( D \) is the small strain consistent tangent operator. The fourth order tensor \( \mathbf{L} \) is defined by:

\[ \mathbf{L} = \frac{\partial \ln \left( \mathbf{B}_{n+1}^{e, \text{trial}} \right)}{\partial \left[ \mathbf{B}_{n+1}^{e, \text{trial}} \right]}, \]  \hfill (4.89)
and the fourth order tensor $B$ is defined by the cartesian components:

$$B_{ijkl} = \delta_{ik} \left( B^e_{n+1} \right)_{jl} + \delta_{jk} \left( B^e_{n+1} \right)_{il}.$$  \hspace{1cm} (4.90)

In the spatial global tangent stiffness, relation (4.88), the fourth order tensor $D$ is material dependent. It means that consistent tangent operator, $D$, is dependent on the material model under study but the other components of spatial tangent stiffness are totally kinematic components, i.e. independent of the material model.

We know that stress is composed of deviatoric stress and hydrostatic pressure:

$$\sigma_{n+1} = s_{n+1} - p_{n+1} \mathbf{I},$$ \hspace{1cm} (4.91)

where, the deviatoric stress is given by:

$$s_{n+1} = 2G \varepsilon^e_{n+1} = 2Gl_d : (\varepsilon^e_{n+1}).$$ \hspace{1cm} (4.92)

The stress deviator could be represented as:

$$s_{n+1} = 2Gl_d : (\varepsilon^e_{n+1} - (\Delta \varepsilon)^P_{n+1}) = 2Gl_d : \varepsilon^{e\text{trial}}_{n+1} - 2Gl_d : (\Delta \varepsilon)^P_{n+1}.$$ \hspace{1cm} (4.93)

The hydrostatic pressure defined with the following relation:

$$p_{n+1} = -\frac{1}{3} tr(\sigma_{n+1}).$$ \hspace{1cm} (4.94)

The tangent operator is given by:

$$D = \frac{d\sigma_{n+1}}{d\varepsilon_{n+1}} = \frac{d\sigma_{n+1}}{d\varepsilon^{e\text{trial}}_{n+1}}.$$ \hspace{1cm} (4.95)

Using relations (4.91) and (4.94), the tangent operator could be written as:

$$\frac{d\sigma_{n+1}}{d\varepsilon_{n+1}} = \frac{ds_{n+1}}{d\varepsilon_{n+1}} - \frac{dp_{n+1}}{d\varepsilon_{n+1}} \mathbf{I}.$$ \hspace{1cm} (4.96)

The first term in the tangent operator which is derivative of the stress deviator in order to strain is given by:

$$\frac{ds_{n+1}}{d\varepsilon_{n+1}} = \frac{d}{d\varepsilon_{n+1}} [2Gl_d : \varepsilon^{e\text{trial}}_{n+1} - 2Gl_d : (\Delta \varepsilon)^P_{n+1}],$$ \hspace{1cm} (4.96)

or equivalently,

$$\frac{ds_{n+1}}{d\varepsilon_{n+1}} = 2Gl_d - \frac{d}{d\varepsilon_{n+1}} [2Gl_d : (\Delta \varepsilon)^P_{n+1}],$$ \hspace{1cm} (4.97)

which can be rewritten in the following from:

$$\frac{ds_{n+1}}{d\varepsilon_{n+1}} = 2Gl_d - 2G \frac{d(\Delta \varepsilon)^P_{n+1}}{d\varepsilon_{n+1}}.$$ \hspace{1cm} (4.97)
Considering equation (4.97), we need to determine the calculate the term \( \frac{d(\Delta \varepsilon)^P_{n+1}}{d\varepsilon_{n+1}} \) which is basically derivative of a second order tensor, \((\Delta \varepsilon)^P_{n+1}\), in order to strain which is a second order, \(\varepsilon_{n+1}\), which results in a fourth order tensor.

According to relation (4.9), the derivative \( \frac{d(\Delta \varepsilon)^P_{n+1}}{d\varepsilon_{n+1}} \) could be written as follows:

\[
\frac{d(\Delta \varepsilon)^P_{n+1}}{d\varepsilon_{n+1}} = \frac{d}{d\varepsilon_{n+1}} \left( \frac{1}{2} \Delta t \left[ \begin{array}{c} \frac{1}{2} \Delta t \varepsilon_{n+1} \end{array} \right] \right) (4.98)
\]

which could be rewritten as follows:

\[
\frac{d(\Delta \varepsilon)^P_{n+1}}{d\varepsilon_{n+1}} = \sqrt{\frac{1}{2}} \Delta t \left( \frac{d|\gamma^P_{n+1}|}{d\varepsilon_{n+1}} \otimes \varepsilon_{n+1} \right) + \sqrt{\frac{1}{2}} \Delta t \varepsilon_{n+1} \frac{d}{d\varepsilon_{n+1}} \left( \frac{s_{n+1}}{|s_{n+1}|} \right) (4.99)
\]

The second term in the right hand side of equation (4.99) could be expanded by making the following:

\[
\frac{d}{d\varepsilon_{n+1}} \left( \frac{s_{n+1}}{|s_{n+1}|} \right) = \frac{1}{|s_{n+1}|} \left( \frac{ds_{n+1}}{d\varepsilon_{n+1}} : s_{n+1} \right) (4.100)
\]

The derivative of the norm of stress deviator in order to strain is given by:

\[
\frac{d|s_{n+1}|}{d\varepsilon_{n+1}} = \frac{1}{|s_{n+1}|} \left( \frac{ds_{n+1}}{d\varepsilon_{n+1}} : s_{n+1} \right) (4.101)
\]

Using relations (4.97), (4.99), (4.100), (4.101) the following relation is obtained:

\[
\frac{ds_{n+1}}{d\varepsilon_{n+1}} + \sqrt{\frac{1}{2}} \Delta t \varepsilon_{n+1} \left[ \frac{1}{|s_{n+1}|} \frac{ds_{n+1}}{d\varepsilon_{n+1}} - \frac{1}{(|s_{n+1}|)^3} \frac{ds_{n+1}}{d\varepsilon_{n+1}} : (s_{n+1} \otimes s_{n+1}) \right] = 2Gd \left( \frac{d|\gamma^P_{n+1}|}{d\varepsilon_{n+1}} \otimes \frac{s_{n+1}}{|s_{n+1}|} \right) (4.102)
\]

According to relation (4.95), we need to have the derivative of the deviatoric stress, \(s_{n+1}\), and hydrostatic stress, \(p_{n+1}\), in order to strain, \(\varepsilon_{n+1}\). Considering relation (4.102), in order to have the derivative of stress deviator in order to strain, it is required to compute \(\frac{ds_{n+1}}{d\varepsilon_{n+1}}\). In order to obtain the required terms, for the tangent operator, we will proceed as presented.

For the sake of notational convenience, the unknowns we have, \(\Delta \varepsilon^P_{n+1}(1), \Delta \varepsilon^P_{n+1}(2), \Delta \varepsilon^P_{n+1}(3), \Delta \varepsilon^P_{n+1}(4)\), are named as shown below:

\[
\begin{align*}
\Delta \varepsilon^P_{n+1}(1) &\rightarrow u(1) \\
\Delta \varepsilon^P_{n+1}(2) &\rightarrow u(2) \\
\Delta \varepsilon^P_{n+1}(3) &\rightarrow u(3) \\
\Delta \varepsilon^P_{n+1}(4) &\rightarrow u(4)
\end{align*}
\] (4.103)
4.3 Consistent tangent operator

Matrix relation (4.104), could be written:

\[
\begin{bmatrix}
    -\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1} \\
    -\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1} \\
    \vdots \\
    -\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}
\end{bmatrix} =
\begin{bmatrix}
    \frac{\partial R_1}{\partial u_1} & \frac{\partial R_1}{\partial u_2} & \frac{\partial R_1}{\partial u_3} & \cdots & \frac{\partial R_1}{\partial u_7} \\
    \frac{\partial R_2}{\partial u_1} & \frac{\partial R_2}{\partial u_2} & \frac{\partial R_2}{\partial u_3} & \cdots & \frac{\partial R_2}{\partial u_7} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    \frac{\partial R_7}{\partial u_1} & \frac{\partial R_7}{\partial u_2} & \frac{\partial R_7}{\partial u_3} & \cdots & \frac{\partial R_7}{\partial u_7}
\end{bmatrix} \begin{bmatrix}
    du_1 \\
    du_2 \\
    du_3 \\
    du_4 \\
    d^{5}P \\
    ds_{n+1} \\
    dp_{n+1}
\end{bmatrix}. \tag{4.104}
\]

Where, the seventh residual equation, \( R_7 \), is given by:

\[
R_7 := p_{n+1} + KI : \varepsilon_{n+1} = 0. \tag{4.105}
\]

Relation (4.104), is rewritten by:

\[
\begin{bmatrix}
    du_1 \\
    du_2 \\
    du_3 \\
    du_4 \\
    d^{5}P \\
    ds_{n+1} \\
    dp_{n+1}
\end{bmatrix} =
\begin{bmatrix}
    C_{1,1} & C_{1,2} & \cdots & C_{1,7} \\
    C_{2,1} & C_{2,2} & \cdots & C_{2,7} \\
    \vdots & \vdots & \ddots & \vdots \\
    C_{7,1} & C_{7,2} & \cdots & C_{7,7}
\end{bmatrix} \begin{bmatrix}
    \frac{\partial R_1}{\partial u_1} : d\varepsilon_{n+1} \\
    \frac{\partial R_1}{\partial u_2} : d\varepsilon_{n+1} \\
    \vdots \\
    \frac{\partial R_1}{\partial u_7} : d\varepsilon_{n+1}
\end{bmatrix}^{-1}. \tag{4.106}
\]

where,

\[
\begin{bmatrix}
    C_{1,1} & C_{1,2} & \cdots & C_{1,7} \\
    C_{2,1} & C_{2,2} & \cdots & C_{2,7} \\
    \vdots & \vdots & \ddots & \vdots \\
    C_{7,1} & C_{7,2} & \cdots & C_{7,7}
\end{bmatrix} =
\begin{bmatrix}
    \frac{\partial R_1}{\partial u_1} & \frac{\partial R_1}{\partial u_2} & \frac{\partial R_1}{\partial u_3} & \cdots & \frac{\partial R_1}{\partial u_7} \\
    \frac{\partial R_2}{\partial u_1} & \frac{\partial R_2}{\partial u_2} & \frac{\partial R_2}{\partial u_3} & \cdots & \frac{\partial R_2}{\partial u_7} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    \frac{\partial R_7}{\partial u_1} & \frac{\partial R_7}{\partial u_2} & \frac{\partial R_7}{\partial u_3} & \cdots & \frac{\partial R_7}{\partial u_7}
\end{bmatrix}^{-1}. \tag{4.107}
\]

Expanding matrix relation (4.106) gives the following system of equations.

\[
\begin{align*}
    du_1 &= C_{1,1}(\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + C_{1,2}(\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + \cdots + C_{1,7}(\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) \\
    du_2 &= C_{2,1}(\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + C_{2,2}(\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + \cdots + C_{2,7}(\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) \\
    du_3 &= C_{3,1}(\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + C_{3,2}(\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + \cdots + C_{3,7}(\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) \\
    du_4 &= C_{4,1}(\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + C_{4,2}(\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + \cdots + C_{4,7}(\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) \\
    d^{5}P &= C_{5,1}(\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + C_{5,2}(\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + \cdots + C_{5,7}(\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) \\
    ds_{n+1} &= C_{6,1}(\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + C_{6,2}(\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + \cdots + C_{6,7}(\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) \\
    dp_{n+1} &= C_{7,1}(\frac{\partial R_1}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + C_{7,2}(\frac{\partial R_2}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) + \cdots + C_{7,7}(\frac{\partial R_7}{\partial \varepsilon_{n+1}} : d\varepsilon_{n+1}) \tag{4.108}
\end{align*}
\]
In order to compute the required unknowns for the tangent operator, \( D \), we need to have the derivatives of the residual equations, \( R_1, R_2, R_3, R_4, R_5, R_6, R_7 \), in order to unknowns, \( \Delta \varepsilon_{n+1}^P(1), \Delta \varepsilon_{n+1}^P(2), \Delta \varepsilon_{n+1}^P(3), \Delta \varepsilon_{n+1}^P(4), \gamma_{i_{n+1}}^P, s_{n+1} \) and \( p_{n+1} \) and also in order to strain \( \varepsilon_{n+1} \). For the state update stage of the solution the derivatives of the first six residual equations, \( R_1, R_2, R_3, R_4, R_5, R_6 \), in order to first six unknowns, \( \Delta \varepsilon_{n+1}^P(1), \Delta \varepsilon_{n+1}^P(2), \Delta \varepsilon_{n+1}^P(3), \Delta \varepsilon_{n+1}^P(4), \gamma_{i_{n+1}}^P, s_{n+1} \), are computed and provided in relations (4.16)-(4.81).

We need to Compute:

- The derivatives of the first six residual equations in order to hydrostatic pressure, \( p_{n+1} \):
  \[
  \frac{\partial R_1}{\partial p_{n+1}} = \frac{\partial R_2}{\partial p_{n+1}} = \frac{\partial R_3}{\partial p_{n+1}} = \frac{\partial R_4}{\partial p_{n+1}} = 0, \quad (4.109)
  \]

- The derivatives of seventh equation, \( R_7 \), in order to all unknowns:
  \[
  \frac{\partial R_5}{\partial p_{n+1}} = -\dot{\gamma}_0 \exp (C_{24}) K_1, \quad (4.110)
  \]

  where,
  \[
  K_1 = \frac{\partial C_{24}}{\partial p_{n+1}}, \quad (4.111)
  \]

  which is given by:
  \[
  K_1 = \frac{-A\alpha T}{1 - \left( \frac{\tau_{n+1}}{s_{n+1}} \right)^{(5/6)}} - \frac{A\tilde{s}_{n+1}}{T} \left( \frac{5}{6} \left( \frac{\tau_{n+1}}{s_{n+1}} \right)^{(-1/6)} K_2 \right), \quad (4.112)
  \]

  where,
  \[
  K_2 = \frac{-\alpha \tau_{n+1}}{s_{n+1}}. \quad (4.113)
  \]

The other derivatives in order to pressure is given below:
\[
\frac{\partial R_6}{\partial p_{n+1}} = 0, \quad \frac{\partial R_7}{\partial p_{n+1}} = 1. \quad (4.114)
\]

The last equation, \( R_7 \), is only dependent on pressure, \( p_{n+1} \), and consequently the derivatives of the last residual equation in order to all unknowns but pressure, \( p_{n+1} \), are zero.
\[
\frac{\partial R_7}{\partial u_1} = \frac{\partial R_7}{\partial u_2} = \frac{\partial R_7}{\partial u_3} = \frac{\partial R_7}{\partial u_4} = \frac{\partial R_7}{\partial u_5} = \frac{\partial R_7}{\partial u_6} = 0. \quad (4.115)
\]
4.3 Consistent tangent operator

The last set of required relations to be determined are the derivatives of the all residual equations in order to strain. It should be emphasized that since strain, \( \varepsilon_{n+1} \), is a second order tensor and the equations are scalar quantities, the derivatives of each residual equation in order to strain result in a second order tensor.

Now, we proceed with the derivatives \( R_1, R_2, R_3, R_4 \) in order to strain:

\[
\frac{\partial R_1}{\partial \varepsilon_{n+1}} = \gamma_{n+1} \sqrt{\frac{1}{2} \Delta t} \frac{\partial}{\partial \varepsilon_{n+1}} (\frac{s_{n+1}(1)}{|s_{n+1}|}),
\]

\[
\frac{\partial R_2}{\partial \varepsilon_{n+1}} = \gamma_{n+1} \sqrt{\frac{1}{2} \Delta t} \frac{\partial}{\partial \varepsilon_{n+1}} (\frac{s_{n+1}(2)}{|s_{n+1}|}),
\]

where,

\[
\frac{\partial s_{n+1}(1)}{\partial \varepsilon_{n+1}^{\text{trial}}} = 2G \begin{bmatrix} \frac{2}{3} \\ \frac{1}{3} \\ 0 \end{bmatrix},
\]

and the next one \( \frac{\partial R_2}{\partial \varepsilon_{n+1}} = \),

\[
\frac{\partial R_3}{\partial \varepsilon_{n+1}} = \gamma_{n+1} \sqrt{\frac{1}{2} \Delta t} \frac{\partial}{\partial \varepsilon_{n+1}} (\frac{s_{n+1}(3)}{|s_{n+1}|}),
\]

where, we have:

\[
\frac{\partial s_{n+1}(2)}{\partial \varepsilon_{n+1}^{\text{trial}}} = 2G \begin{bmatrix} \frac{2}{3} \\ \frac{1}{3} \\ 0 \end{bmatrix},
\]

Now, it is the turn of \( \frac{\partial R_3}{\partial \varepsilon_{n+1}} = \),

\[
\frac{\partial R_4}{\partial \varepsilon_{n+1}} = \gamma_{n+1} \sqrt{\frac{1}{2} \Delta t} \frac{\partial}{\partial \varepsilon_{n+1}} (\frac{s_{n+1}(4)}{|s_{n+1}|}),
\]

where,

\[
\frac{\partial s_{n+1}(4)}{\partial \varepsilon_{n+1}^{\text{trial}}} = 2G \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \\ 0 \end{bmatrix},
\]
4.3 Consistent tangent operator

The norm of stress deviator is given by:

\[ ||s_{n+1}|| = \sqrt{s_{n+1}(1)s_{n+1}(1) + s_{n+1}(2)s_{n+1}(2) + 2s_{n+1}(3)s_{n+1}(3) + s_{n+1}(4)s_{n+1}(4)}. \]  

(4.124)

The derivative of the fifth equation in order to strain is given in:

\[ \frac{\partial R_5}{\partial \varepsilon_{n+1}} = -\dot{\gamma}_0 \exp \left[ -\frac{A\tilde{s}_{n+1}}{\theta} \left( 1 - \frac{\tau_{n+1}}{s_{n+1}} \right)^{\frac{5}{6}} \right] \times, \]

(4.125)

Relation (4.125) could be rewritten as:

\[ \frac{\partial R_5}{\partial \varepsilon_{n+1}} = -\dot{\gamma}_0 \exp \left[ -\frac{A\tilde{s}_{n+1}}{\theta} \left( 1 - \frac{\tau_{n+1}}{s_{n+1}} \right)^{\frac{5}{6}} \right] \times, \]

\[ -\frac{A\tilde{s}_{n+1}}{\theta} \times \frac{\partial}{\partial \varepsilon_{n+1}} \left[ -\left( \frac{\tau_{n+1}}{s_{n+1}} \right)^{\frac{5}{6}} \right], \]

(4.126)

or in a more simplified form:

\[ \frac{\partial R_5}{\partial \varepsilon_{n+1}} = -\dot{\gamma}_0 \exp \left[ -\frac{A\tilde{s}_{n+1}}{\theta} \left( 1 - \frac{\tau_{n+1}}{s_{n+1}} \right)^{\frac{5}{6}} \right] \times, \]

\[ +\frac{A\tilde{s}_{n+1}}{\theta} \times \frac{\partial}{\partial \varepsilon_{n+1}} \left[ \left( \frac{\tau_{n+1}}{s_{n+1}} \right)^{\frac{5}{6}} \right], \]

(4.127)

where \( \tau_{n+1} \) is an equivalent stress defined by:

\[ \tau_{n+1} = \sqrt{\frac{1}{2}s_{n+1} : s_{n+1}}. \]  

(4.128)

Using relations (4.127) and (4.128), we can have:

\[ \frac{\partial R_5}{\partial \varepsilon_{n+1}} = -\frac{5\sqrt{2}}{6} \dot{\gamma}_0 AG \left( \frac{\tau_{n+1}}{s_{n+1}} \right)^{-\frac{1}{6}} s_{n+1} \exp \left\{ -\frac{A\tilde{s}_{n+1}}{\theta} \left( 1 - \frac{\tau_{n+1}}{s_{n+1}} \right)^{\frac{5}{6}} \right\}. \]

(4.129)

The other derivatives are provided below:

\[ \frac{\partial R_6}{\partial \varepsilon_{n+1}} = 0, \]

(4.130)

\[ \frac{\partial R_7}{\partial \varepsilon_{n+1}} = KI. \]

(4.131)
Chapter 5

Numerical examples

This chapter presents some numerical examples through which the capability of the model to characterize the typical deformation behaviour of polymers is assessed and also the efficiency of the derived and implemented algorithm is shown.

The material under study is polymethylmethacrylate (PMMA). The material properties required for performing the simulations are taken from (Boyce et al., 1988). The material properties are tabulated in Table (5.1). Different examples including compression on a cube, cylinder compression, notched bar compression and necking of a round bar are selected to be analysed.

<table>
<thead>
<tr>
<th></th>
<th>$E$</th>
<th>$\nu$</th>
<th>$s_0$</th>
<th>$\alpha$</th>
<th>$\gamma_0$</th>
<th>$A$</th>
<th>$h$</th>
<th>$s_{ss}$</th>
<th>$R$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA</td>
<td>2300</td>
<td>0.37</td>
<td>88E+6</td>
<td>0.2</td>
<td>1.13E+11</td>
<td>167E-06</td>
<td>900E+06</td>
<td>77E+06</td>
<td>8.3143</td>
</tr>
</tbody>
</table>

5.1 Compression of a cube (plane strain compression)

In this section, a compression test on a cube is performed which can be approximated in 2D as plane strain compression. The geometry and mesh of the problem is shown in Figure (5.1). The specimen is spatially discretized with 128 quadrilateral eight noded elements with reduced four integration Gauss points. The stress strain curve for the plane strain compression test is given in Figure (5.2). In Figure (5.2), the typical deformation behaviour of glassy polymers which includes initial linear elastic, yield, post-yield softening could be observed. It should be emphasized that the reason for not-seeing the final hardening regime in the deformation is that the hardening stress
5.1 Compression of a cube (plane strain compression)

Figure 5.1: The geometry and mesh of the plane strain compression test.

Figure 5.2: The stress-strain curve for the compression of the cube.

is not considered in this study.
In order to assess the performance and numerical efficiency of the derived and implemented algorithm, the convergences are going to be checked. In Table (5.2), the local convergence of the problem at two different load increments is shown.
From Table (5.2), it can be concluded that the state update algorithm is derived
5.2 Cylinder upsetting (axisymmetric compression)

This section presents results of a compression test on a cylinder. The Geometry is the same as the one shown in Figure (5.1) and the same material properties but under axisymmetric condition is used for the simulation. Figure (5.3), shows stress-strain curve for the cylinder upsetting simulation. In order the check the numerical efficiency, the convergence of the cylinder upsetting simulation are investigated. Table (5.3) presents local convergence (state update) for two different load increments.

### Table 5.2: Local convergence table for cube compression simulation

<table>
<thead>
<tr>
<th>Iteration number</th>
<th>The value of the residual at local level</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Increment (6)</td>
</tr>
<tr>
<td>1</td>
<td>0.383915E-05</td>
</tr>
<tr>
<td>2</td>
<td>0.295615E-10</td>
</tr>
<tr>
<td>3</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.3: The stress-strain curve for the compression of the cylinder.
Table 5.3: Local convergence table for cylinder compression simulation

<table>
<thead>
<tr>
<th>Iteration number</th>
<th>Increment (6)</th>
<th>Increment (35)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.779533</td>
<td>0.532699</td>
</tr>
<tr>
<td>2</td>
<td>0.010266E-04</td>
<td>0.880138E-02</td>
</tr>
<tr>
<td>3</td>
<td>0.312095E-08</td>
<td>0.059476E-04</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>0.740346E-05</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>0.737990E-07</td>
</tr>
</tbody>
</table>

5.3 Notched bar compression

The next example is a notched bar under uniaxial compression. The geometry and mesh of the problem is shown in Figure (5.4). The specimen is spatially discretized with 350 eight noded quadrilateral elements with reduced four integration Gauss points. Figure (5.5) depicts contour plot of the effective stress in whole specimen when ten percent of the deformation is applied. Figure (5.6) shows contour plot of the effective stress in whole specimen at twenty percent of the deformation. Effective stress in the specimen when 30 percent of the deformation is applied is shown in Figure (5.7). When half of the deformation has proceed, the effective stress is given in Figure (5.8). The final contour plot, depicted in Figure (5.9), shows the effective stress at the end of the deformation.
5.3 Notched bar compression

Figure 5.5: Contour plot of effective stress at ten percent of the deformation.

Figure 5.6: Contour plot of effective stress at twenty percent of the deformation.

Figure 5.7: Contour plot of effective stress at thirty percent of the deformation.
5.3 Notched bar compression

Figure 5.8: Contour plot of effective stress at half of the deformation.

Figure 5.9: Contour plot of effective stress at the end of the deformation.
Chapter 6

Conclusions and suggestions for future research

In this thesis, a constitutive model was developed based on BPA model, which is one of the most well-known constitutive models proposed for polymers. Finite Element Method was used to solve the equilibrium equation. The integration algorithm of the model was presented for finite element implementation. The well-known Newton-Raphson method is used at state update (local) level and also equilibrium (global) level to solve the non-linear system of equations. Hence, in this thesis we have used two important numerical methods, namely finite element method and Newton-Raphson method, to deal with equilibrium equations of solid polymers. It is worth emphasizing that, there might be a possibility to improve the integration algorithm of the model by reducing the system of equations to another system of equations with reduced number of equations or even to a single scalar equation.

According to the results presented in chapter five of this work, it can be concluded that the BPA based model can predict the typical polymeric materials behavior. In order to have an idea of the capabilities and drawbacks of the model predictions, it is required to have a wide range of experimental results under different deformation modes. Comparing simulations and experimental results will help to realize the accuracy of the model predictions and also the necessity of required changes and modifications to the model. Considering all the remarks provided above, the suggestions for the future research can be summarized as follows:

- Checking the possibility of modification of the integration algorithm
- Making some comparisons with existing experimental results
- Proposing some applicable modifications to the constitutive relations in order to improve model predictions
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and postyield behaviour and corresponding structure of poly(methyl methacrylate).


