3 Finite Element Analysis as an Engineering Tool

Chapter Outline

3.1 Introduction

Polymer mechanics is the study of how the mechanical behavior of polymers depend on external load environments. It is a broad subject that provides tools to engineers and scientist interested in understanding the behavior of polymer components and how their performance can be predicted and optimized. This chapter provides a broad overview of different approaches and techniques that can be used when studying polymer mechanics problems, and as indicated in the title, the focus is on the use of the finite element (FE) method.

Polymeric materials have during the last few decades been gradually transformed from being conceived as low-budget, low-technology materials—exemplified by expression such as “it is just a plastic”—to highly reliable and advanced materials with excellent mechanical properties. One of the driving forces for this transformation has been the development of a better understanding of polymer behavior and how polymer components should be designed. In other word, experimental and theoretical polymer

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mechanics have paved the way for new and improved uses of polymers.

Designing components and products using polymers require specific knowledge about their behavior. This is important since their mechanical behavior is very different than traditional engineering metals, see Table 3.1. One of the main challenges of polymer mechanics is that it is a multi-disciplinary subject that has strong ties to mechanical engineering, material science, bioengineering, and chemical engineering—all of which are core

Table 3.1 Overview of Differences in Properties of Polymers and Metals

Polymers	Metals
Exhibit nonlinear viscoelastic behavior when deformed at room temperature	Exhibit elastic-plastic behavior when deformed at room temperature
Often contain both amorphous and semi-crystalline domains	Crystalline microstructure[a]
Visco-plastic deformation driven by macromolecular reorganization	Plastic deformation driven by dislocation motion and twinning
At temperatures close to room temperature, the material response is very strongly dependent on deformation rate and temperature	Rather weak dependence on deformation rate and temperature at temperatures close to room temperatures
The maximum usage temperature is never more than 300 °C and is often less than 100 °C	Can be used in very high temperature applications (higher than 800 °C)
Do not corrode	Corrodes in an aggressive environment
Can dissolve in an aggressive environment	Generally impervious to solvents

[a] *By using specialized manufacturing methods it is possible to create metals that are amorphous.*

subjects of most educational institutions. Polymer mechanics, as a subject, draws heavily on these disciplines, although the emphasis of polymer mechanics in this context is perhaps most strongly connected with mechanical engineering.

There are different analytical techniques that can be used when studying the mechanical behavior of polymers. The traditional approach, and until about 30 years ago the only approach, is to use closed-form analysis to study deformations and stresses and how these influence ultimate properties such as fatigue and fracture.

The development of the FE method and computers have revolutionized not only polymer mechanics, but all fields of component design and analysis. The reason for this is that the FE method enables direct analysis of complex geometries with relatively little effort, problems that cannot even be solved using traditional closed-form analytical techniques. A summary of different classes of analysis techniques, and their strengths and weaknesses is presented in Table 3.2.

As indicated in this table, closed-form analysis, when applicable, provides the most detailed information. For example, using this technique it is possible to determine not only the stress state for a given imposed deformation state but also the mathematical dependence of how geometry and load history directly influence the stress state.

FE tools have reached a high level of maturity and are widely used in both academia and industry. The easy access to commercial FE codes has created both great possibilities to solve advanced problems, and to some extent reduced the need for costly experimental tests. However, this computational modeling approach also presents serious challenges since the FE programs, albeit being easy to use, can provide inaccurate and misleading results if not used properly. One of the overall aims of this text is to assist the creation and selection of FE models and analysis techniques for polymer problems.

3.1.1 Required Inputs for FEA

To perform an FE simulation, or indeed any stress analysis calculation, there are three different types of inputs that need to

Table 3.2 Summary of Different Analysis Techniques, Their Strengths and Limitations, and How They Can Be Applied to Polymer Mechanics Problems

Analysis Method	Strengths	Limitations
Closed-form calculation using a simple material model (e.g., linear elasticity)	+ Computationally efficient + Provides the mathematical relationship between deformation and stress	− Only applicable to simple geometries
FE simulation using a simple material model	+ Captures nonlinear geometric effects − Easy to calibrate material model	− Simple material models often do not give accurate results
FE simulation using an advanced material model	+ Captures nonlinear geometric effects + Can very accurately capture the material response	− More difficult to calibrate material model − More computationally costly

be specified, see Figure 3.1. Note that these inputs are also needed for traditional closed-form solution methods.

The fundamental problem of polymer mechanics can be written in mathematical form as a boundary value problem (BVP), with governing equations for: compatibility, constitutive response, and equilibrium. More details of these equations are given in Chapter 4. One of the overall themes of this book is that of the three different types of input to the FE models: (1) geometry; (2) loading and boundary conditions (BC); and (3) material behavior; it is the specification of the material behavior that is typically most challenging.

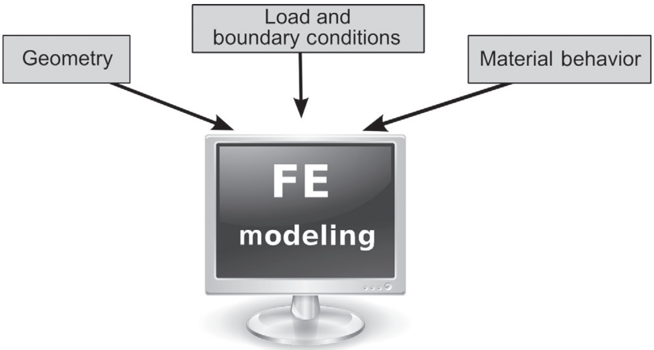

Figure 3.1 Inputs needed for FE analysis.

3.2 Types of FEA

The FE method can be described as a numerical tool for solving ordinary and partial differential equations over nontrivial geometric domains. In practice, finite element analysis (FEA) can be divided into two different categories: implicit and explicit simulations, see Table 3.3. FEA can also be used to study eigenfrequencies and eigenmodes of deformation for a component or system.

As mentioned, one of the most difficult steps in an FE simulation is to specify the material model. A material model is here defined as a constitutive equation and a corresponding set of material parameters:

Constitutive model + **Material parameters** = **Material model**

FE software contains a library of different constitutive equations that can be chosen, but the material parameters are typically not provided and the selection of constitutive models that are available is typically targeted to metals. There are generally only a limited set of constitutive models that are suitable for predicting the deformation behavior of polymers. One way to get around this is to use an external user material subroutine (UMAT) to define the material behavior, see Chapter 10 for more details.

Table 3.3 Comparison Between Implicit and Explicit FEA

Implicit Analysis	Explicit Analysis
Solves the equilibrium equations at each time step	Solves the problem using Newton's law of motion
Good for static problems	Good for short duration dynamic problems
Is numerically stable	Is only numerically stable for small time increments
If the FE software finds a solution, that solution is likely to have small numerical errors	Often easy to find a solution, but care is needed to find a solution with small numerical errors
Contact problems are sometimes difficult to handle	Good at handling problems with contact

3.3 Review of Modeling Techniques

Most polymer mechanics problems can be divided into two main categories: predictions of deformation behavior and predictions of failure events. A common approach is to start with a deformation analysis to determine the magnitudes and distributions of stress and strain, and then, if needed, use this information as part of a predictive failure analysis. The following subsections provide brief examples of these modeling types. More detailed presentations of the modeling theories are given in the following chapters.

3.3.1 Deformation Modeling

A key component of polymer mechanics analyses involves determining the deformation response as a function of applied loads. The following two examples illustrate common problems that a polymer mechanist may be exposed to.

Example: Thermomechanical Deformations of a Threaded Connection Gasket.
One example of a deformation model is a PTFE gasket in a threaded connection for high pressure pipelines, see the illustration in Figure 3.2. The pipeline shown in this figure is used to transport gases at temperatures between 20 °C and 200 °C. The two parts of the pipeline are threaded together, and the primary seal to prevent gas leakage is created by a metal-to-metal seal. In this example, a PTFE gasket is used as a secondary seal to reduce the risk of gas leaks. The gasket used in this seal is made from PTFE filled with 10 vol% glass fibers.

The manufacturer of the pipeline wanted to reduce the number of costly experiments and enable faster design evaluations. To achieve these goals it was decided to develop an FE model of the PTFE gasket and threaded connection, see Figure 3.3. In this figure, the interior pipe, the gasket, and the exterior pipe have been separated vertically to better illustrate the geometry.

The goal of the analysis was to predict the amount of residual sealing force between the PTFE gasket and the interior and exterior pipes as a function of time, temperatures, and seal design. During the assembly of the threaded connection, the gasket it exposed to very large deformations and pressures. It is

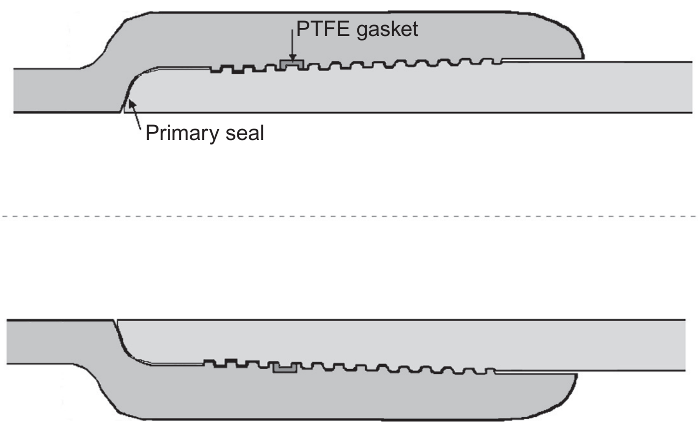

Figure 3.2 Cross-section of a pipeline with a threaded connection containing a PTFE gasket as a secondary seal.

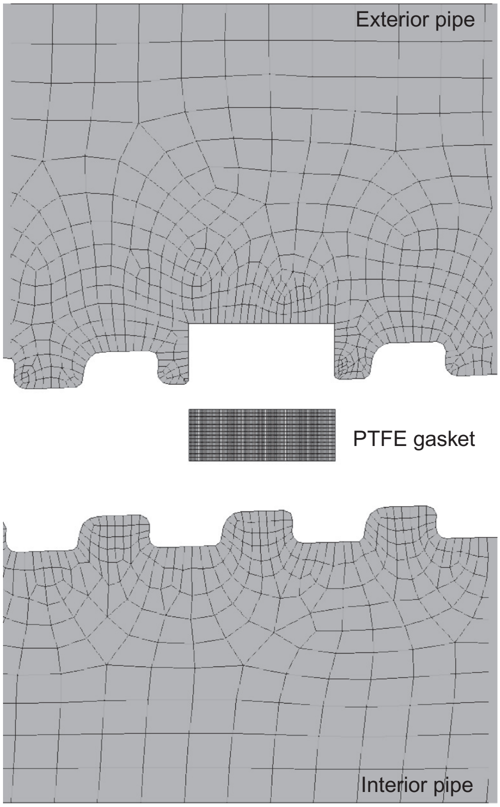

Figure 3.3 Details of the FE mesh close to the PTFE gasket.

therefore necessary to use a constitutive model capable of predicting the large-strain time-dependent thermomechanical behavior of the PTFE. To accomplish this, an advanced material model specifically developed for PTFE was used (the Dual Network Fluoropolymer [DNF] model [1], see Section 8.4). The DNF model is not yet a built-in feature of commercial FE codes, but have been implemented as a UMAT in Abaqus, ANSYS, and LS-DYNA [2]. The results presented below were obtained using Abaqus/Standard.

The first step in this project was to experimentally characterize the nonlinear response of the gasket material. This testing included uniaxial monotonic and cyclic loading at different temperatures, volumetric compression experiments, and a multiaxial small punch test [3]. The second step was to calibrate the constitutive model to the experimental data and to validate the material model by comparison to the small punch data (see Section 2.3.2). After the DNF model had been calibrated and validated, it could be used to simulate the deformation behavior of the PTFE gasket at the temperatures and deformation states of interest.

One example of the results that were obtained from the stress analysis are presented in Figures 3.4 and 3.5.

Figure 3.4 shows contours of Mises stress (in MPa) in the gasket region. It is clear that the stresses in the metal pipes are very high and that the PTFE gasket has been significantly deformed.

A more detailed picture of the stress state in the PTFE gasket is shown in Figure 3.5.

In summary, by calibrating an advanced material model to the PTFE gasket material it is possible to use FE simulations to

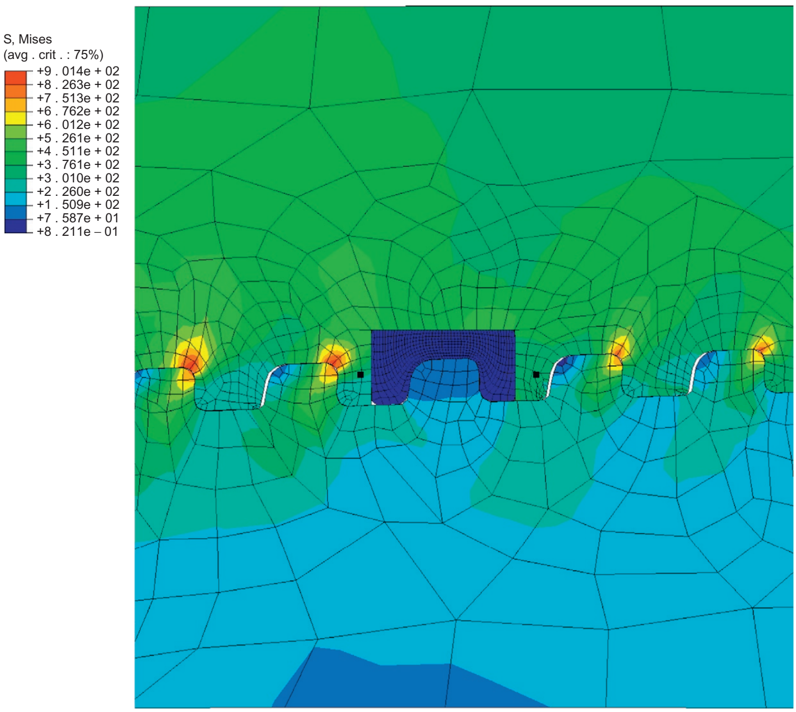

Figure 3.4 Contours of Mises stress (in MPa) in the threaded connection and the PTFE gasket. A mesh refinement study is needed in order to make sure the mesh is refined enough.

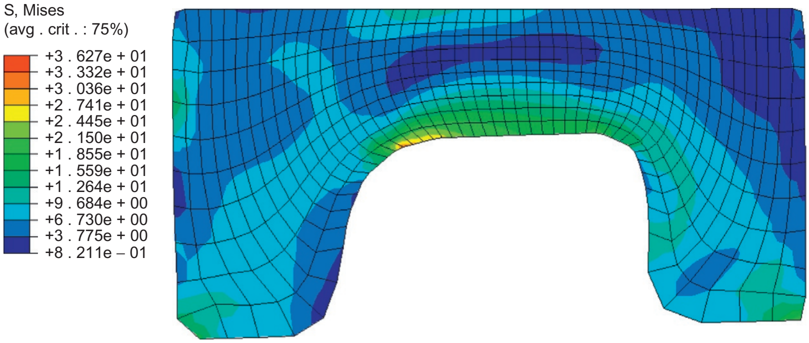

Figure 3.5 Details of the Mises stress (in MPa) in the gasket.

directly predict the sealing capability as a function of seal design and loading conditions.

Example: Deformation of a Flex Circuit Pressure Sensor. Flex circuit pressure sensors are used in a wide variety of applications, including touch displays and child seat sensors in car seats. This type of sensor typically consists of a top and bottom layer separated by a spacer layer. The actual sensing region consists of a cavity in the spacer layer, see Figure 3.6. The top and bottom layers are often made from a thermoplastic, and the spacer layer is often made from an adhesive. The bottom surface of the top layer and the top surface of the bottom layer are made conducting by adding conducting particles, such as carbon black. The applied pressure can be determined by measuring the resistance between the top and bottom layers.

This example illustrates the use of the FE method to examine the influence of sensor curvature on the sensor performance. The electrical resistance is directly related to the contact area, so the

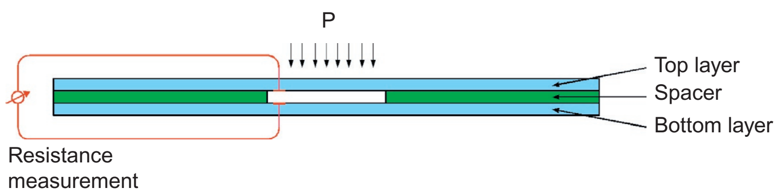

Figure 3.6 Schematic side view of a flex circuit pressure sensor.

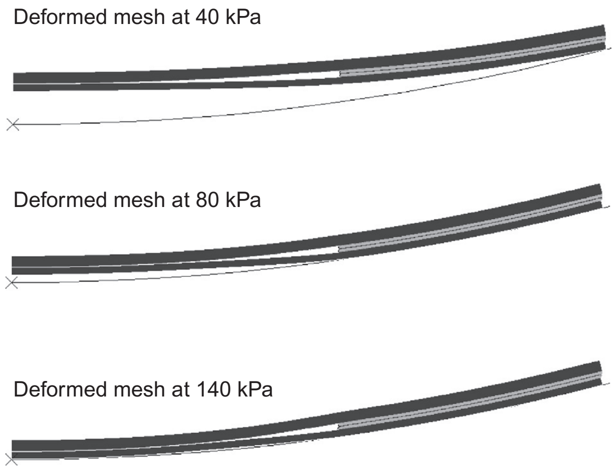

Figure 3.7 Deformed shapes of the flex circuit pressure sensor at different applied pressures.

goal of these simulations is to determine the contact area as a function of applied pressure and curvature.

The performance of the pressure sensor will depend on the electric stability and creep characteristics of the materials in the sensor, and how the pressure is applied. In this case, the behavior of each layer of the sensor was first experimentally examined. Then appropriate constitutive models were calibrated to each material. One example of the type of simulations that were performed to study the pressure sensor design is shown in Figure 3.7. Here, an axisymmetric representation of the sensor was placed on a rigid surface with a given radius of curvature. This approach enabled a direct determination of the influence of radius of curvature and applied pressure on the contact area.

3.3.2 Failure Modeling

The perhaps most obvious criterion when designing a part is that it should not fail in normal use during its intended lifetime. Here, *failure* is defined as material failure or fracture by the creation of new material surfaces and parts. Failure is a collective term for both fracture and rupture, where rupture is a special

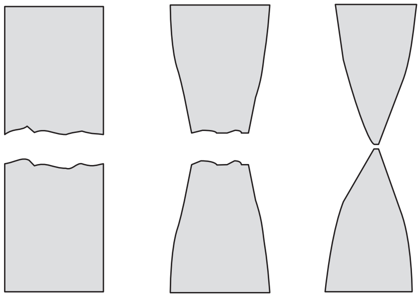

Figure 3.8 Schematic representation of different failure modes.

failure mode in which failure occurs by localized thinning to a point, see Figure 3.8. Both fracture and rupture can occur either by monotonic or cyclic loading. Note, rupture is a somewhat uncommon event that is only seen in the most ductile polymers.

Failure can be caused by different mechanisms and be of different types; for example, monotonic overloading, cyclic fatigue, or wear. For polymers, failure is also often caused by a combination of mechanical loads and material degradation due to environmental exposure. This combination of mechanical loads and material degradation is commonly referred to as environmental stress cracking (ESC).

The following examples illustrate the analysis of common failure scenarios.

Example: Failure of a Water Filter.
Failure of polymer components can often be attributed to one or more of the following reasons:

- material selection;
- part design;
- manufacturing processes; and
- service/environmental conditions.

This example illustrates a failure that was caused by a combination of material selection and part design. The failed component in this case is a water purification system. The water filter consisted

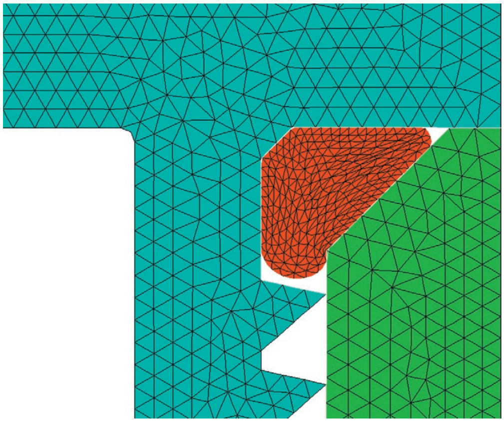

Figure 3.9 Details of a two-dimensional axisymmetric FE model of the tank (green), connector head (blue), and o-ring (red).

of a water inlet, a tank filled with the purification agent, and a water outlet. In this case, the water filter frequently failed by the connector head breaking off from the tank. The bottom threaded region of the connector head was made of acrylonitrile butadiene styrene (ABS). By examining the fracture surfaces of failed parts it was clear that the fracture initiation site was the top thread of the connector head.

To study the failure mode a two-dimensional axisymmetric FE model was created to assess the stress level in the head, see Figure 3.9. This figure shows that in its assembled state, an interior o-ring that is located between the connector head and the tank becomes severely distorted.

An example of the stress-contours in the connector head in the assembled state is shown in Figure 3.10.

The figure shows that there is a stress concentration near the threads of the plastic head. The maximum Mises stress was 65% of the yield stress of the polymer. The conclusion of the stress analysis is that the material was not defective, either the design needs to be modified to reduce the stress or a different material should be used.

Example: Failure of Corrugated Hose.

A corrugated PTFE hose was used to transport liquid SO_3 (sulfur trioxide) at a chemical plant. The hose consisted of an exterior

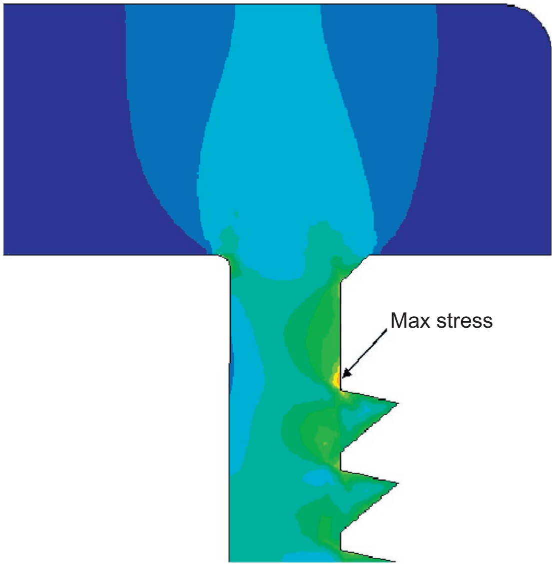

Figure 3.10 Contours of Mises stress in the connector head in the assembled state.

layer of braided stainless steel with a corrugated PTFE liner inside Over time, a small amount of SO_3 diffused through the PTFE liner and reached the load-carrying stainless steel braid which gradually corroded due to its interaction with the SO_3 and exterior water.

Eventually, all stainless steel corroded away in one section, and the axial load and internal pressure were applied directly to the PTFE liner. In the section where the steel had been corroded away, the PTFE liner could not take the applied loads and failed, causing a release of SO_3, and environmental problems.

An FEA was performed to better understand the failure events and what the internal pressure was at the time of the failure. Two examples illustrating the results from this analysis are presented in Figures 3.11 and 3.12.

Figure 3.11 shows the deformed shape of a cross-section of the hose, and contours of the maximum principal stress. In this simulation, the applied temperature was 100 °C, the internal pressure was 120 kPa, and the results are shown 1 s after the application of the load.

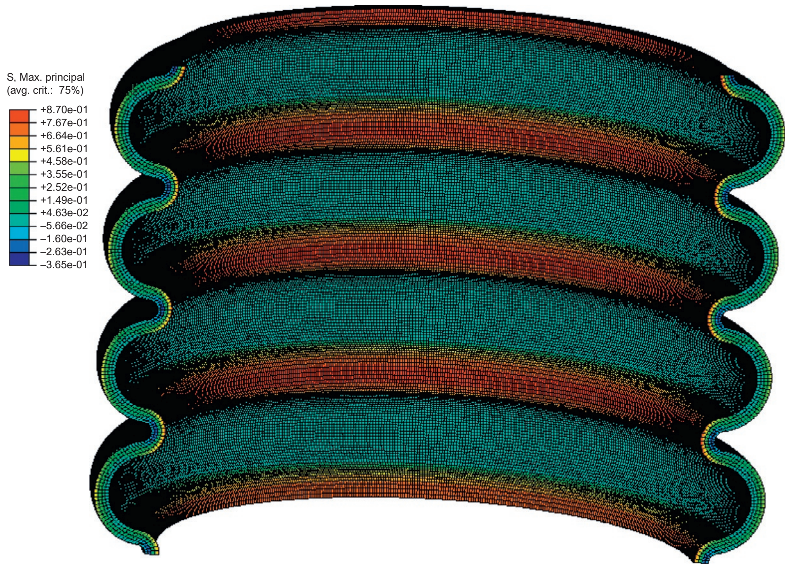

Figure 3.11 Contours of maximum principal stress (in MPa): temperature $T = 100\,°C$, $P = 120$ kPa, $F = 0$ N, loading time $t = 1$ s.

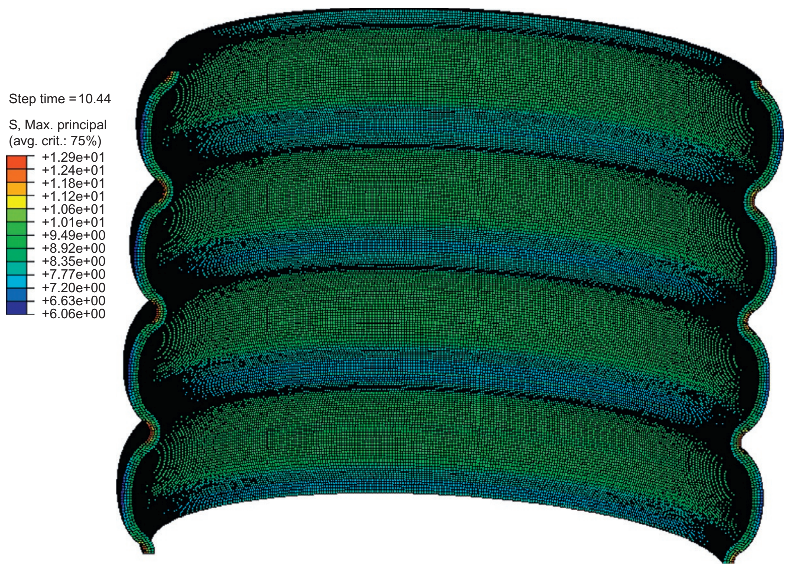

Figure 3.12 Contours of maximum principal stress (in MPa): temperature $T = 100\,°C$, $P = 120$ kPa, $F = 0$ N, loading time $t = 60$ s.

Figure 3.12 shows the results from the same load scenario, except that the results in this case are for a time of 60 s after the application of the load. It is clear that the liner undergoes large viscoplastic deformations at this temperature and applied pressure. Also, note that the location of the maximum stress changes as a function of time from the internal surface to the exterior surface.

3.4 Exercises

1. What are some of the key differences between polymers and metals?
2. What are the three required input types for an FE simulation?
3. What are some of the key differences between explicit and implicit FE simulations? When is it appropriate to perform an implicit simulation, and when is it appropriate to perform an explicit simulation?
4. Describe the difference between a material model and a constitutive model.
5. What are the four most common reasons a polymer component might fail?

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