Accurate Finite Element Simulations of PTFE Components

Jorgen Bergstrom, Ph.D.
jbergstrom@veryst.com

Veryst Engineering, LLC

May 17, 2012
Outline

- PTFE background
- Goals
- Experimental data
- Material models
- Calibration procedure
- Results
- Conclusions
PTFE Background

• Polytetrafluoroethylene (PTFE) is a fluoropolymer with unique properties:
  – very hydrophobic
  – very non-reactive due to high F-C bond strength
  – discovered in 1938
  – melting point: 327°C = 621°F
  – lowest friction coefficient of any polymer
  – excellent dielectric properties
  – cannot be crosslinked
  – used in medical devices such as vascular grafts, and many sealing applications

PTFE is the only known surface to which a gecko cannot stick
Goal

• The mechanical response of fluoropolymers is highly non-linear

• Find a suitable material model that can capture the observed experimental response!
Uniaxial Compression

- Uniaxial compression at 2 strain rates, followed by unloading
- The material recovers quickly during unloading
Uniaxial Tension

- quick relaxation also at small $\varepsilon$
Comparison of absolute value of tension and compression stress-strain behavior.

The compressive response is very different than the tensile response!
Cyclic Volumetric Compression

![Graph showing cyclic volumetric compression with true stress vs. true strain. The graph includes a line labeled "triaxial (strain rate=-1e-6) (experimental)." There is also a diagram of a specimen being compressed.]
Experimental Data

- Small Punch (0.008 mm/s) (experimental)
# Material Models Investigated

- Neo-Hookean hyperelasticity  
  **Abaqus Built-In**
- Isotropic hardening plasticity
- Drucker-Prager plasticity
- Dual Network Fluoropolymer (DNF) model **PolyUMod**
- Three Network (TN) model
Neo-Hookean

- Simplest possible hyperelastic model
- Only two parameters \((\mu, \kappa)\)

\[
\Psi = \frac{\mu}{2} (I_1^* - 3) + \frac{\kappa}{2} (J - 1)^2
\]

\[
\sigma = \frac{\mu}{J} \text{dev}[b^*] + \kappa(J - 1)I
\]

\[
\lambda = \frac{L}{L_0}
\]

\[
\sigma_{\text{uniax}} = \mu \left( \lambda^2 - \frac{1}{\lambda} \right)
\]

\[
\sigma_{\text{planar}} = \mu \left( \lambda^2 - \frac{1}{\lambda^2} \right)
\]

\[
\sigma_{\text{biaxial}} = \mu \left( \lambda^2 - \frac{1}{\lambda^4} \right)
\]
Isotropic Hardening Plasticity

- Mises yield surface with an associated flow rule
- Linear unloading until reverse plasticity

*Hyperelastic
*Plastic
*Rate Dependent

$$E, \nu, \varepsilon_i^p, \sigma_i^y$$

$$(i = 1, 2, 3, \ldots, N)$$

$$D, n$$
Drucker Prager Plasticity

- For frictional materials like granular solids
- Can predict different yield strength in tension and compression
- Can incorporate strain-rate dependence and progressive failure
- Rate-dependent yield:

\[ R = 1 + \left( \frac{\varepsilon_p}{D} \right)^{1/n} \]

a) Linear Drucker-Prager: \( F = t - p \tan \beta - d = 0 \)

b) Hyperbolic: \( F = \sqrt{(d' \tan \beta - p_i) + q^2} - p \tan \beta - d' = 0 \)

c) Exponent form: \( F = aq^2 - p - p_i = 0 \)
**Dual Network Fluoropolymer (DNF) Model**

*PolyUMod implementation available for both Abaqus/Standard and Abaqus/Explicit, Mechanics of Materials, vol 37, pp. 899-913, 2005 (J. Bergstrom, L. Hilbert)
Three Network Model


The material model contains 3 network components:
Three Network Model (TNM)

- Large strain response controlled by entropic resistance
- Initial viscoplastic response captured using two separate energy activation mechanisms corresponding to amorphous and semicrystalline domains

Crosslinked, 110°C
Material Model Calibration

Step 1: Add Experimental Data

(movie)
Results: Neo-Hookean

The NH model does not work well!
Results: Isotropic Hardening Plasticity

Average: R2 = 0.40

Material Model: EP 1

NMAD Fitness = 61.8

NMAD Fitness = 31
Results: Isotropic Hardening Plasticity

Average: R2 = 0.40

NMAD Fitness = 34.7

NMAD Fitness = 21.8
Results: Drucker Prager

Average: $R^2 = 0.56$

NMAD Fitness = 34.6

NMAD Fitness = 18.2
Results: Drucker Prager

Average: $R^2 = 0.56$
Results: DNF Model

Average: 
\( R^2 = 0.82 \)

NMAD Fitness = 16.8

NMAD Fitness = 15
Results: DNF Model

Average: $R^2 = 0.82$

NMAD Fitness = 13.1

NMAD Fitness = 2.42
Results: Three Network Model

![Graphs showing stress vs. strain for different models and conditions, with annotations for compression-cyclic and tension-larger, and average R² = 0.86.](image)

**Average:**

\[ R^2 = 0.86 \]
Results: Three Network Model

Average: $R^2 = 0.86$
Results: Performance

Benchmark Test 1: 1298 C3D8R elements, Abaqus/Standard

Benchmark Test 2: 1298 CPE4R elements, Abaqus/Standard
Results: Performance

- Best
- Worst
- TNM
- DNF
- Drucker-Prager
- J2-plasticity (isotropic)
- Neo-Hookean

Normalized Run Time vs. R² Value
Results: Performance

Normalized Mean Absolute Difference:

\[ f(\sigma^p, \sigma^e) = \frac{\langle |\sigma^p - \sigma^e| \rangle}{\langle |\sigma^e| \rangle} \]
Conclusions

• Fluoropolymers is an important thermoplastic with a highly non-linear response

• The experimentally observed behavior can be accurately captured using the Three Network (TN) model or the Dual Network Fluoropolymer (DNF) models

• The TN and DNF models are available for both Abaqus/Standard and Abaqus/Explicit