ASPECTS OF A FINITE STRAIN CONSTITUTIVE MODEL FOR SEMICRYSTALLINE POLYMERS

Thesis submitted by
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List of Publications

Throughout the progression of this research there have been several international conference presentations and international journal articles. The chapters of this thesis largely resemble these publications following the plan outline here.

Chapter 2 was presented in part at the Australian and Korean Rheology Conference, 2005 (AKRC05). The chapter has been published in largely unaltered form under the citation

> Holmes, D.W., Loughran, J.G., Suehrcke, H. (2007) Constitutive Model for Large Strain Deformation of Semicrystalline Polymers, *Mech. Time-Depend. Mater.*, **10**, 281-313, `http://dx.doi.org/10.1007/s11043-007-9023-8`.

Chapter 3 was presented at the World Congress on Computational Mechanics 2006 (WCCM VII). The chapter has been submitted for journal publication in largely unaltered form under the citation

> Holmes, D.W., Loughran, J.G. (submitted June 2007) Numerical Aspects Associated with the Implementation of a Finite Strain, Elasto-viscoelastic-viscoplastic Constitutive Theory in Principal Stretches, *Int. J. Numer. Meth. Engng.*

Chapter 4 has been submitted for journal publication in largely unaltered form under the citation

> Holmes, D.W., Loughran, J.G. (2007) Theoretical Aspects of the Testing of Elasto-viscoelastic-viscoplastic Materials, *Polym. Test.*, `http://dx.doi.org/10.1016/j.polymertesting.2007.10.002`.

Chapter 5 has been presented in part at Computational Techniques and Applications Conference 2006 (CTAC-06) and the accompanying paper has been accepted for publication in the conference proceedings under the citation

> Holmes, D.W., Loughran, J.G. (accepted March 2007) A Theory for the Isolation of the Complex Deformation Characteristics of Nonlinear Viscoelastic Materials, *ANZIAM J. (CTAC-06)*.

Statement on the Contribution of Others

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Abstract

In this thesis, the development of a constitutive model for the finite strain deformation of semicrystalline polymers is presented. It reports on the formulation and numerical implementation of the model and the theoretical aspects of the associated experimental testing and parameter estimation.

Within both academia and industry to date, there exists no single constitutive model for semicrystalline polymers that is broadly accepted as representing the general case. This is in spite of the relatively complete scientific understanding of the material's response and the increasing use of such materials where structural loading can be significant. Numerical representation of such materials conventionally involves over-simplification of response, largely necessitated by the limitations of current experimental testing methods. A complex constitutive theory is only as powerful as the experimental method from which its parameters are fit. As such, the objective of this research was to develop a complete, generalized constitutive theory for semicrystalline polymers with a corresponding testing methodology that enables its practical use within industry.

The constitutive model selected can be characterized by a parallel combination of elastic, viscoelastic and viscoplastic model elements which most closely represents the complete deformation behavior of semicrystalline polymers in the pre-necking region ($\varepsilon < 15\%$). The accompanying mathematics are formulated for 3D, finite strain and are based on thermodynamic dissipation in keeping with conventional continuum mechanics methodology. Strain hardening has been found to be of importance within the viscoplastic element. The parallel configuration of the three model elements facilitates the decoupled algorithmic treatment of each response. This has been carried out in principal space, given the assumption of isotropy, making practical both its numerical implementation and the physical determination of model parameters. A strategy analogous to classical return mapping is used for

solution of the viscoelastic evolution while a new, principal space, closest point projection return mapping algorithm has been developed for solution of the viscoplastic evolution, accounting for isotropic strain hardening. The consistent algorithmic tangential modulus is formulated to ensure quadratic convergence of the whole implicit finite element procedure.

The computational model has been verified through a series of simple finite element tests involving combinations of large strain normal and shear loadings, and large rigid body rotations. Several example problems have been solved as demonstration of the models versatility.

Using the developed model, a study using numerical simulations of uniaxial and biaxial tensile testing methods has been carried out. Through this study it has been possible to develop an experimental methodology to isolate the component stress contributions from each of the three deforming modes as well as subset separation of viscous, yield, and isotropic hardening stresses for viscoplasticity. Via conventional optimisation procedures and an additionally developed iterative procedure for the viscoelastic response, this testing methodology makes possible the full specification of the model parameter set. Verification of the testing methodology was done via comparison between the calculated test curves, and values output directly from the numerical simulations.

The model proposed in this thesis corresponds to a general account of semicrystalline polymer constitutive response, possessing capabilities not accounted for previously in theories within the literature. Perhaps the most significant outcome from this work is the experimental data processing methodology that allows such a complex model to be accurately and practically fit to real materials. Being able to better predict the loaded response of semicrystalline polymers is critical for their continued and increased use in circumstances where structural loads are possible.

Contents

List of Tables

List of Figures