

# Computational Modeling of Polymer Composites

*A Study of Creep and Environmental Effects*

---



*Dedication*  
**To Our Mothers**



# Computational Modeling of Polymer Composites

*A Study of Creep and Environmental Effects*

**SAMIT ROY**

Department of Aerospace Engineering and Mechanics  
University of Alabama  
Tuscaloosa, Alabama

**J. N. REDDY**

Department of Mechanical Engineering  
Texas A&M University  
College Station, Texas

**CRC Press**

Boca Raton • London • New York • Washington, D.C.

---

**Library of Congress Cataloging-in-Publication Data**

---

Roy, Samit and Reddy, J. N.

Computational Modeling of Polymer Composites

Samit Roy and J. N. Reddy.

Bibliography: p

Includes index

ISBN 0-000-00000-0

1. Computational Modeling
2. Polymer Composites. I. Title.

TA405.F423 1988

620.1'12—dc19

This book contains information obtained from authentic and highly regarded sources. Reprinted material is quoted with permission, and sources are indicated. A wide variety of references are listed. Reasonable efforts have been made to publish reliable data and information, but the author and the publisher cannot assume responsibility for the validity of all materials or for the consequences of their use.

Neither this book nor any part may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopying, microfilming, and recording, or by any information storage or retrieval system, without prior permission in writing from the publisher.

The consent of CRC Press LLC does not extend to copying for general distribution, for promotion, for creating new works, or for resale. Specific permission must be obtained in writing from CRC Press LLC for such copying.

Direct all inquiries to CRC Press LLC, 2000 N.W. Corporate Blvd., Boca Raton, Florida 33431.

**Trademark Notice:** Product or corporate names may be trademarks or registered trademarks, and are used only for identification and explanation, without intent to infringe.

---

**Visit the CRC Press Web site at [www.crcpress.com](http://www.crcpress.com)**

---

© 2013 by CRC Press LLC

No claim to original U.S. Government works

International Standard Book Number 0-000-00000-0

Printed in the United States of America 1 2 3 4 5 6 7 8 9 0

Printed on acid-free paper

# Contents

---

Preface . . . . .	xv
<b>1. General Introduction and Equations of Solid Mechanics . . . . .</b>	<b>1</b>
1.1 Introduction . . . . .	1
1.2 Vectors and Tensors . . . . .	2
1.2.1 Definitions . . . . .	2
1.2.2 Components of Vectors and Tensors . . . . .	2
1.2.3 Summation Convention . . . . .	4
1.2.4 The Del Operator . . . . .	5
1.2.5 Transformations of Components . . . . .	6
1.3 Equations of Solid Mechanics . . . . .	9
1.3.1 Introduction . . . . .	9
1.3.2 Kinematics . . . . .	10
1.3.3 Compatibility Equations . . . . .	13
1.3.4 Stress Vector and Stress Tensor . . . . .	14
1.3.5 Equations of Motion . . . . .	16
1.3.6 Constitutive Relations: Hooke's Law . . . . .	17
1.3.7 Linear Viscoelasticity . . . . .	21
1.4 Energy Principles of Solid Mechanics . . . . .	25
1.4.1 Introduction and Concept of Work Done . . . . .	25
1.4.2 The Principle of Virtual Displacements . . . . .	26
1.4.3 The Principle of Minimum Total Potential Energy . . . . .	29
1.5 Summary . . . . .	31
References . . . . .	31
<b>2. A Review of the Finite Element Method . . . . .</b>	<b>33</b>
2.1 Introduction . . . . .	33
2.2 Linear Plane Elasticity Problems . . . . .	34

2.2.1	Governing Equations . . . . .	34
2.2.2	Finite Element Approximation . . . . .	36
2.2.3	Virtual Work Statement . . . . .	37
2.2.4	Finite Element Model . . . . .	38
2.3	Finite Element Models of Nonlinear Continua . . . . .	40
2.3.1	Introduction . . . . .	40
2.3.2	Strain and Stress Measures . . . . .	41
2.3.3	Principle of Virtual Displacements . . . . .	43
2.3.4	Total Lagrangian Formulation . . . . .	44
2.3.5	Updated Lagrangian Formulation . . . . .	45
2.3.6	2-D Finite Element Models . . . . .	46
2.3.6.1	Total Lagrangian formulation . . . . .	46
2.3.6.2	Updated Lagrangian formulation . . . . .	47
2.4	Numerical Integration . . . . .	48
2.4.1	Preliminary Comments . . . . .	48
2.4.2	Coordinate Transformations . . . . .	48
2.4.3	Integration over a Master Rectangular Element . . . . .	52
2.4.4	Integration over a Master Triangular Element . . . . .	53
2.4.5	Numerical Integration over Three-Dimensional Elements . . . . .	55
2.5	Two-Dimensional Finite Elements . . . . .	56
2.5.1	Properties of Approximation Functions . . . . .	56
2.5.2	Linear Triangular Element . . . . .	56
2.5.3	Linear Rectangular Element . . . . .	58
2.6	Three-Dimensional Finite Elements . . . . .	61
2.6.1	Hexahedral (Brick) Elements . . . . .	61
2.6.2	Tetrahedral Elements . . . . .	61
2.6.3	Prism Elements . . . . .	63
2.7	Summary . . . . .	65
	References . . . . .	65



<b>3. Finite Element Models of Linear Viscoelastic Materials</b> . . . . .	<b>67</b>
3.1 Introduction . . . . .	67
3.2 Linear Viscoelastic Formulation . . . . .	67
3.2.1 Introduction . . . . .	67
3.2.2 Uniaxial Stress State . . . . .	69
3.2.3 Multiaxial Stress State . . . . .	71
3.2.4 Three-Dimensional Viscoelastic Constitutive Relations . . . . .	76
3.3 Finite Element Analysis . . . . .	79
3.3.1 Finite Element Model . . . . .	79
3.3.2 Example Problems . . . . .	80
3.3.2.1 Creep and recovery of axisymmetric viscoelastic rod . . . . .	80
3.3.2.2 Response of an axisymmetric viscoelastic rod to cyclic load . . . . .	83
3.3.2.3 Response of a three-dimensional viscoelastic rod to cyclic load . . . . .	85
3.3.2.4 Delayed failure in a linear viscoelastic material . . . . .	85
3.4 Summary . . . . .	93
References . . . . .	93
<b>4. Finite Element Analysis of Diffusion in Polymer and Polymer Matrix Composites</b> . . . . .	<b>95</b>
4.1 Introduction . . . . .	95
4.1.1 Preliminary Comments . . . . .	95
4.1.2 Diffusion in a Polymer . . . . .	97
4.2 Modeling of Moisture Diffusion . . . . .	99
4.2.1 Governing Equations . . . . .	99
4.2.2 Finite Element Formulation . . . . .	100
4.2.3 Solution of Nonlinear Equations . . . . .	102
4.2.3.1 Direct iteration scheme . . . . .	102
4.2.3.2 Newton's iteration scheme . . . . .	103
4.2.4 Axisymmetric Diffusion Problems . . . . .	103

4.2.4.1 Preliminary comments . . . . .	103
4.2.4.2 Finite element model . . . . .	104
4.2.5 Numerical Examples . . . . .	105
4.2.5.1 One-dimensional linear Fickian diffusion in a polymer film . . . . .	105
4.2.5.2 Two-dimensional Fickian diffusion in an orthotropic material . . . . .	107
4.2.5.3 Hygrothermal stresses in two-dimensional Fickian diffusion in an orthotropic material . . . . .	111
4.3 Diffusion with Time-Varying Diffusivity . . . . .	113
4.3.1 Introduction . . . . .	113
4.3.2 Governing Equations . . . . .	113
4.3.3 Analytical Solution . . . . .	114
4.3.4 Variational (Weak) Form . . . . .	116
4.3.5 Finite Element Model . . . . .	116
4.3.6 A Numerical Example . . . . .	117
4.4 Summary . . . . .	119
References . . . . .	119
<b>5. Finite Element Models of Nonlinear Viscoelastic Materials . . . . .</b>	<b>123</b>
5.1 Introduction . . . . .	123
5.2 Uniaxial Stress State . . . . .	124
5.3 Multiaxial Stress State . . . . .	127
5.4 Constitutive Relations for Three-Dimensional Viscoelasticity . . . . .	133
5.5 Finite Element Model . . . . .	136
5.6 Example Problems of Nonlinear Viscoelasticity . . . . .	137
5.6.1 Analysis of Adhesive Coupons . . . . .	137
5.6.2 Isothermal Creep and Recovery in an Epoxy Adhesive . . . . .	140
5.6.3 Analysis of a Model Joint . . . . .	144
5.6.4 Analysis of a Composite Single Lap Joint . . . . .	150

5.6.5 Nonlinear Isochronous Creep in an Axisymmetric Rod . . . . .	153
5.7 Delayed Failure . . . . .	156
5.7.1 Uniaxial Formulation . . . . .	156
5.7.2 Multiaxial Formulation . . . . .	157
5.7.3 Example: A Butt Joint . . . . .	159
5.8 Summary . . . . .	162
References . . . . .	162
<b>6. Finite Element Analysis of Nonlinear Diffusion in Polymers . . . . .</b>	<b>167</b>
6.1 Introduction to Nonlinear Fickian Diffusion . . . . .	167
6.2 Background on Nonlinear Diffusion Analysis . . . . .	168
6.3 Newton–Raphson Technique for Solving Nonlinear Diffusion Problem . . . . .	169
6.4 Iterative Solution Procedure . . . . .	170
6.5 Examples of Nonlinear Diffusion Problems . . . . .	171
6.5.1 Diffusion in a Semi-Infinite Media . . . . .	171
6.5.2 Gas Transport in Uniaxially Stretched Polystyrene . . . . .	173
6.5.3 Analysis of a Butt Joint Including Moisture Diffusion . . . . .	176
6.6 Summary . . . . .	186
References . . . . .	186
<b>7. Non-Fickian Solvent Diffusion in a Solid with Large Dilatation 189</b>	
7.1 Introduction . . . . .	189
7.2 Governing Equations . . . . .	190
7.3 Swelling (Dilatation) due to Solvent Ingress in an Orthotropic Solid . . . . .	191
7.3.1 Governing Equations . . . . .	191
7.3.2 Finite Element Formulation . . . . .	193
7.3.3 Time-Integration using $\theta$ -Family of Approximation . . . . .	195
7.3.4 The Newton Iteration Scheme . . . . .	195

7.3.5 Numerical Example: Diffusion in a One-Dimensional Bar with Large Dilatation . . . . .	196
7.3.6 Effective Diffusivity and Diffusivity Correction Factor . . . . .	200
7.3.7 Calculation of Shear Stresses . . . . .	202
7.4 Summary . . . . .	204
References . . . . .	204
<b>8. A Coupled Hygrothermal Cohesive Layer Model for Simulating Debond Growth in Bimaterial Interfaces . . . . .</b>	<b>205</b>
8.1 Preliminary Comments . . . . .	205
8.2 Introduction . . . . .	205
8.3 Cohesive Layer Model Development . . . . .	207
8.4 Derivation of Consistent Diffusivities . . . . .	212
8.5 Cohesive Layer Diffusion Boundary Conditions . . . . .	212
8.6 Cohesive Work of Separation . . . . .	213
8.7 Numerical Implementation . . . . .	214
8.8 Finite Element Model Verification . . . . .	215
8.8.1 Comparison with Analytical Solution for a DCB Specimen . . . . .	215
8.8.2 Modification of DCB Solution (Modified Williams' Model) . . . . .	219
8.9 Comparison Between Analytical Solution and Finite Element Results . . . . .	222
8.10 Simulation of Debond Growth due to Bond Degradation: Wedge Test Simulation . . . . .	228
8.11 Summary . . . . .	234
References . . . . .	234
<b>9. A Viscoelastic Cohesive Layer Model for Prediction of Interlaminar Shear Strength of Carbon/Epoxy Composites . . . . .</b>	<b>237</b>
9.1 Introduction . . . . .	237
9.2 Background . . . . .	238

9.3 Finite Element Modeling . . . . .	238
9.4 A Multi-Scale Viscoelastic Cohesive Layer Formulation Including Damage Evolution . . . . .	239
9.4.1 Governing Equations . . . . .	239
9.4.2 Damage Evolution Law . . . . .	241
9.4.3 Determination of Principal Stretch . . . . .	242
9.4.4 Damage Initiation Criterion . . . . .	243
9.5 Hydrolysis of Epoxy Resins in a Polymer Composite . . . . .	244
9.5.1 Introduction . . . . .	244
9.5.2 Mechanism-Based Modeling of Degradation Due to Hygrothermal Aging in Polymer Composites . . . . .	244
9.5.3 Calculation of Moisture Degradation Parameter $r$ . . . . .	245
9.5.4 Derivation of Internal State Variable for Moisture-Induced Degradation . . . . .	245
9.5.5 Modeling of Strength Degradation due to Hygrothermal Effects . . . . .	247
9.5.6 Delamination Failure at the Interface between Adjacent Lamina in a Unidirectional Carbon/Epoxy Laminate . . . . .	248
9.6 Results and Discussion . . . . .	248
9.6.1 Finite Element Simulation of Short Beam Shear Experiments . . . . .	248
9.6.2 A Sensitivity Study of the Effect of Displacement Rate on Cohesive Law . . . . .	250
9.6.3 Verification of Model Prediction with Test Data for Interlaminar Shear Strength . . . . .	252
9.7 Summary . . . . .	254
References . . . . .	255
<b>10. A Multi-Scale Viscoelastic Cohesive Layer Model for Predicting Delamination in High Temperature Polymer Composites . . . . .</b>	<b>257</b>
10.1 Introduction . . . . .	257
10.2 Double Cantilever Beam (DCB) Experiment . . . . .	260

10.2.1 Specimen Preparation and DCB Specimen Geometry . . . . .	260
10.2.2 Experimental Method . . . . .	261
10.3 Viscoelastic Cohesive Layer Model . . . . .	261
10.3.1 Preliminary Comments . . . . .	261
10.3.2 Damage Evolution Law for the Micromechanical RVE . . . . .	262
10.4 Extraction of Cohesive Law from Experimental Data Through $J$ -Integral . . . . .	263
10.5 Evaluation of Damage Evolution Law . . . . .	265
10.6 Numerical Results . . . . .	268
10.7 Summary . . . . .	271
References . . . . .	272
<b>Index . . . . .</b>	<b>275</b>

# Preface

---

Most significant developments in engineering in the last three decades have been in the area of materials modeling. Foremost among these developments have been the development of polymeric materials and their use in smart materials and structures, functionally graded materials (FGMs), composites, and nanoscience and technology – each topic deserves to be treated in a monograph by itself.

The focus for the present book is the education of the individual who is interested in gaining a good understanding of the theories and associated finite element models of elastic and viscoelastic response of polymers and polymer composites. The subject is truly an interdisciplinary one, where chemists, material scientists, chemical engineers, mechanical engineers, and structural engineers contribute to the overall product. The courses offered at universities and the books published on polymer composites are of three types: material science, mechanics, and numerical simulations. The present book belongs to the *computational mechanics* category in that it covers both mechanics aspects as well as computational aspects.

The motivation for the present book has come from many years of the authors' research and teaching in composite materials and from the fact there does not exist a book that covers computational modeling of polymers and polymeric composites. The book is largely based on the authors' original works in the subject area over the last three decades.

Some mathematical preliminaries, equations of anisotropic elasticity, and virtual work principles and variational methods are reviewed in Chapter 1. A reader who has a knowledge of these topics may skip this chapter and go directly to Chapter 2, where an introduction to the finite element method is presented.

The primary journey of the book begins with Chapter 3, where finite element analysis of viscoelastic materials is presented. Both linear and nonlinear viscoelastic models are considered. Chapter 4 is dedicated to diffusion process in polymers and polymer matrix composites. Chapter 5 covers finite element models of viscoelastic materials. Both uniaxial and multiaxial cases are considered, and delayed failure is discussed. In Chapter 6, finite element analysis of nonlinear Fickian diffusion process in polymers is studied, while non-Fickian diffusion of polymers is discussed in Chapter 7.

Chapter 8 is devoted to a study of coupled hygrothermal cohesive layer model for simulating debond growth in bimaterial interfaces. A viscoelastic cohesive layer model for prediction of interlaminar shear strength of carbon/epoxy composites is

presented in Chapter 9. Finally, Chapter 10 deals with a multi-scale viscoelastic cohesive layer model for predicting delamination in high temperature polymer composites.

The book is suitable as a reference for engineers and scientists working in industry and academia, and it can be used as a textbook in a graduate course on theory and/or finite element analysis of polymers and polymeric composites. An introductory course on mechanics of materials as well as on the finite element method may prove to be helpful. While the authors tried to minimize any errors in the book, it is likely that they missed some. The authors request readers to send their comments and corrections to *sroy@eng.ua.edu* or *jnreddy@tamu.edu*.

The authors express their gratitude to Dr. Vinu Unnikrishnan and Mr. Priyank Upadhyaya (University of Alabama) for their invaluable help in the preparation of the manuscript. The authors also express their sincere thanks to Mr. Jonathan Plant, Senior Editor (Engineering) at CRC Press, for his support in producing this book.

Samit Roy  
*Tuscaloosa, Alabama*

J. N. Reddy  
*College Station, Texas*



## About the Authors

---

**Samit Roy** is the William D. Jordan Chair Professor of Aerospace Engineering and Mechanics at University of Alabama, Tuscaloosa. Before moving to an academic position, he was a Senior Research Engineer at the Southwest Research Institute (SWRI), San Antonio, Texas. Dr. Roy has authored 60 journal papers, 11 book chapters, and more than 80 conference papers. Professor Roy's research interest is directed toward multiscale modeling and failure prediction of fiber reinforced polymer composites and structural adhesives subjected to environmental conditions, using the finite element method. His research centers around the development of mechanism-based multiscale structural durability models that would accurately predict long-term performance of materials based on data from accelerated short-term tests. He is also actively involved in the application and simulation of nanostructured reinforcements in enhancing performance of composite materials. At SWRI, he has worked on numerous research projects, including several NASA and Air Force funded projects on the use of polymer matrix composites (PMC) for cryogenic storage as well as for high-temperature supersonic airframe. He was an invited panelist at the Workshop on Composites for Extremely Cold Temperatures and Extraterrestrial Applications, Fairbanks, Alaska, organized by National Science Foundation in August 2004. He was a plenary speaker at the Composites Durability Conference organized jointly by NSF-Cambridge University in September 2007. He was the recipient of Outstanding Teaching Awards and Faculty Excellence Awards at UMR in 1999 and 2000. Dr. Roy is a Fellow of the American Society of Mechanical Engineers and an Associate Fellow of the American Institute of Aeronautics and Astronautics (AIAA), and he was the elected chairman of the AIAA Materials Technical Committee in 2009. He is a member of the editorial boards of *Polymer and Polymer Composites* and *Mechanics of Advanced Materials and Structures* journals. A more complete resume with links to journal papers can be found at <http://unix.eng.ua.edu/~sroy>.

**J. N. Reddy** is a University Distinguished Professor, Regents Professor, and the Holder of Oscar S. Wyatt Endowed Chair at Texas A&M University, College Station. He is the author of more than 485 journal papers and 18 books on composite materials, plates and shells, and the finite element method. Dr. Reddy is recognized by **ISI Highly Cited Researchers** with more than 10,000 citations and *h*-index greater than 50 (the *h*-index as per Google Scholar is 60). Professor Reddy is the recipient of numerous awards including the Walter L. Huber Civil Engineering Research Prize of the American Society of Civil Engineers (ASCE), the Worcester Reed Warner Medal and the Charles Russ Richards Memorial Award of the American Society of Mechanical Engineers (ASME), the 1997 Archie Higdon Distinguished Educator Award from the American Society of Engineering Education, the 1998 Nathan M. Newmark Medal from the American Society of Civil Engineers, the 2000 Excellence in the Field of Composites from the American Society of Composites, and the 2003 Computational Solid Mechanics Award from the U.S. Association of Computational Mechanics. Dr. Reddy received honorary degrees (Honoris Causa) from the Technical University of Lisbon, Portugal, in 2009 and Odlar Yurdu University, Azerbaijan, in 2011. Professor Reddy is a Fellow of AIAA, ASCE, ASME, the American Academy of Mechanics, the American Society of Composites, the U.S. Association of Computational Mechanics, the International Association of Computational Mechanics, and the Aeronautical Society of India. Professor Reddy is the Editor-in-Chief of *Mechanics of Advanced Materials and Structures*, *International Journal of Computational Methods in Engineering Science and Mechanics*, and *International Journal of Structural Stability and Dynamics*; he also serves on the editorial boards of more than two dozen other journals. A more complete resume with links to journal papers can be found at <http://isihighlycited.com/> or <http://www.tamu.edu/acml>.

