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*Editors*

# Flexible Polymer Chain Dynamics in Elongational Flow

Theory  
and  
Experiment

 Springer

# Flexible Polymer Chains In Elongational Flow Theory And Experiments

**Roman Boulatov**



## **Flexible Polymer Chains In Elongational Flow Theory And Experiments:**

Flexible Polymer Chains in Elongational Flow Tuan Q. Nguyen, Hans-Henning Kausch, 2012-12-06 The behavior of polymer solutions in simple shear flows has been the subject of considerable research in the past. On the other hand, reports on polymers in elongational flow have appeared comparatively recently in the literature. Elongational flow with an inherent low vorticity is known to be more effective in extending polymer chains than simple shear flow and thus is more interesting from the point of view of basic molecular chain dynamics at high deformation and applied polymer science: rheology, fiber extrusion, drag reduction, flow through porous media. Undoubtedly, one landmark in the field of polymer dynamics in elongational flow was the notion of critical strain rate for chain extension, initially put forward by A. Peterlin in 1966 and later refined into the coil stretching transition by P. G. de Gennes and H. Hinch in 1974. In the two decades which followed, significant progress in the understanding of chain conformation in strong flow has been accomplished through a combination of advances in instrumentation, computation techniques, and theoretical studies. As a result of the multidisciplinary nature of the field, information on polymer chains in strong flow is accessible only from reviews and research papers scattered in disparate scientific journals. An important objective of this book is to remedy that situation by providing the reader with up-to-date knowledge in a single volume. The editors therefore invited leading specialists to provide both fundamental and applied information on the multiple facets of chain deformation in elongational flow. **Practical Aspects of Chemical**

**Engineering** Marek Ochowiak, Szymon Woźniowski, Michał Doligalski, Piotr Tomasz Mitkowski, 2018-02-07 This book focuses on Chemical Engineering and Processing, covering interdisciplinary innovation technologies and sciences closely related to chemical engineering, such as computer image analysis, modelling, and IT. The book presents interdisciplinary aspects of chemical and biochemical engineering interconnected with process system engineering, process safety, and computer science.

**Polymer Dynamics in Dilute Media** Shikha Somani, 2011 Polymers undergo a sharp coil-to-stretch conformational transition in extension-dominated flows when the strain rate exceeds a critical value. Dramatic change in flow behavior is known to occur at the coil stretch transition, making it useful for several commercial applications. Despite decades of study, this phenomenon remains surrounded with controversy as the effect of solvent properties and fluid flow elements on this transition is not fully understood. In this work, we present a study of the coil stretch transition and related hysteresis phenomenon using stochastic computer simulations. We first investigate the effect of solvent quality on the coil stretch transition using Brownian dynamics simulations. Unlike experiments, which are plagued with problems related to polydispersity of polymers and inaccurate control over flow profiles, simulations offer a powerful platform to systematically study the effect of solvent quality while keeping all other parameters in the system constant. The system consists of a polymer subjected to planar elongational flow in both theta solvents and good solvents. The polymer is represented by a bead-spring chain model undergoing elongational flow. Solvent-mediated effects such as fluctuating hydrodynamic interactions (HI) and

excluded volume EV are included rigorously Conformational hysteresis is understood in terms of a 1 D energy landscape theory with an activation energy barrier for transition At steady state depending upon the flow rate the energy landscape can either have one or two energy wells An energy landscape with one well corresponds to the coiled state at low flow rate and stretched state at high flowrate The double well landscape corresponds to the hysteretic regime where both coiled and stretched conformational states coexist across the ensemble population A key factor in determining the effect of solvent quality is the use of a proper measure of solvent quality In almost all earlier studies the effect of molecular weight on solvent quality has been neglected producing inconsistent results Here the solvent quality is quantified carefully such that the effect of molecular weight and temperature is taken into account Contrary to earlier findings it is observed that with improvement in solvent quality the chains unravel faster and the critical strain rate at which the coil to stretch transition takes place decreases Furthermore the solvent quality has a profound effect on the scaling of the critical strain rate with molecular weight and on both the transient and steady state properties of the system Universal functions are shown to exist for the observed dynamic and static properties which will prove useful in determining the operating parameters for experiments In particular the ratio of the two different relaxation times longest relaxation time and zero shear rate viscosity is found to be a universal function of solvent quality independent of molecular weight The relaxation times both the longest relaxation time and the zero shear rate viscosity increase while the critical strain rate is found to decrease with solvent quality Next the study of conformational hysteresis is extended to more complicated 3 D flows to understand the effect of flow vorticity on this phenomenon Heretofore there has been no systematic methodology for studying the dynamical interactions between polymer molecules and elementary flow patterns in three dimensional flows Such a framework is essential not just for gaining valuable insights into the physics of complex fluids at a fundamental level but it is also crucial for various important applications like turbulent drag reduction where the underlying physical mechanisms involve dynamical interactions between polymers and turbulence fine scale flow features Such a study is presented here to provide a framework to interpret complex fluid phenomenon in terms of elementary flow patterns We investigate the conformational hysteresis using rigorous Brownian dynamics simulations and specifically explore the effect of flow vorticity on the lifetime and width of the hysteresis window in 3 D flows A systematic procedure is developed with careful eigenvalue analysis to explore the sole effect of vorticity on polymer dynamics keeping the principal strain rate fixed It is observed that the hysteresis width shrinks due to increase in flow vorticity irrespective of the flow type bi extensional bi compressional spiral inwards spiral outwards etc This is further traced to the alignment of eigenvectors with the principal eigenvector direction leading to enhanced fluctuations Vorticity is found to have a significant effect on both the transient and the steady state properties Understanding the effect of vorticity on polymer conformational hysteresis can further help in understanding the fundamental processes in complex flows

Surface Science and Adhesion in Cosmetics K. L. Mittal,H. S. Bui,2021-03-08 Activity in the arena of surface chemistry

and adhesion aspects in cosmetics is substantial but the information is scattered in many diverse publications media and no book exists which discusses surface chemistry and adhesion in cosmetics in unified manner This book containing 15 chapters written by eminent researchers from academia and industry is divided into three parts Part 1 General Topics Part 2 Surface Chemistry Aspects and Part 3 Wetting and Adhesion Aspects The topics covered include Lip biophysical properties and characterization use of advanced silicone materials in long lasting cosmetics non aqueous dispersions of acrylate copolymers in lipsticks cosmetic oils in Lipstick structure chemical structure of the hair surface surface forces and interactions AFM for hair surface characterization application of AFM in characterizing hair skin and cosmetic deposition SIMS as a surface analysis method for hair skin and cosmetics surface tensiometry approach to characterize cosmetic products spreading of hairsprays on hair color transfer from long wear face foundation products interaction of polyelectrolytes and surfactants on hair surfaces cosmetic adhesion to facial skin and adhesion aspects in semi permanent mascara lipstick adhesion measurement     Polymer Chain Scission in Extensional and Turbulent Flows and Implications for Friction Drag Technologies Siva A. Vanapalli,2006     Soft Materials John R. Dutcher,Alejandro G. Marangoni,2004-10-01 Representing the wide breadth academic disciplines involved in this ever expanding area of research this reference provides a comprehensive overview of current scientific and technological advancements in soft materials analysis and application Documenting new and emerging challenges in this burgeoning field Soft Materials is a unique and outsta     **Journal of Rheology** ,2005     **Journal of Experimental Biology** ,2006     Tailoring of Nanocomposite Dielectrics Toshikatsu Tanaka,Alun S. Vaughan,2016-11-03 This book illustrates interfacial properties preparation characterization devices and applications from the standpoint of nano interfacial tailoring Since the primary focus of the book is on the use of nanocomposite dielectrics in electrical applications chapters are devoted to directly relevant topics such as surface and bulk breakdown processes However the mechanisms that underpin such behavior are not unique Therefore the book also addresses related topics that range from the chemistry of polymer and nanocomposite degradation to the simulation of charge transport dynamics in disordered materials thereby presenting a multi and interdisciplinary approach to the area It will serve as a practical handbook or graduate textbook and is supplemented by ample number of illustrations case studies practical examples and historical perspectives     **Structure of Turbulence and Drag Reduction** Albert Gyr,2012-12-06 In 1976 a similar titled IUTAM Symposium Structure of Turbulence and Drag Reduction was held in Washington However the progress made during the last thirteen years as well as the much promising current research desired a second one this year In Washington drag reduction by additives and by direct manipulation of the walls compliant walls and heated surfaces were discussed In the meantime it became evident that drag reduction also occurs when turbulence is influenced by geometrical means e g by influencing the pressure distribution by the shape of the body airfoils or by the introduction of streamwise perturbances on a body riblets In the recent years turbulence research has seen increasing attention being focused on the investigation of

coherent structures mainly in Newtonian fluids We all know that these structures are a significant feature of turbulent flows playing an important role in the energy balance in such flows However their place in turbulence theories as well as the factors influencing their development are still poorly understood Consequently the investigation of phenomena in which the properties of coherent structures are altered provides a promising means of improving our understanding of turbulent flows in general

*Brownian Dynamics Simulations of Flowing Isolated Polymer Molecules in Solution Near Surfaces* Manish Chopra, 2001

Experimental Studies of Polymer Chain Conformation in Flow Ellen Cheng-Chi Lee, 1998

**Polymer Translocation** M. Muthukumar, 2016-04-19 Polymer translocation occurs in many biological and biotechnological phenomena where electrically charged polymer molecules move through narrow spaces in crowded environments Unraveling the rich phenomenology of polymer translocation requires a grasp of modern concepts of polymer physics and polyelectrolyte behavior Polymer Translocation discussed

The Science and Technology of Flexible Packaging Barry A. Morris, 2022-07-23

*The Science and Technology of Flexible Packaging Multilayer Films from Resin and Process to End Use* Second Edition provides a comprehensive guide on plastic films in flexible packaging covering scientific principles materials properties processes and end use considerations Sections discuss the science of multilayer films in a concise and impactful way presenting the fundamental understanding required to improve product design material selection and processes In addition the book includes information on why one material is favored over another and how film or coating affects material properties Descriptions and analysis of key properties of packaging films are provided from engineering and scientific perspectives With essential scientific insights best practice techniques environmental sustainability information and key principles of structure design this book provides information aids in material selection and processing how to shorten development times and deliver stronger products and ways to enable engineers and scientists to deliver superior products with reduced development time and cost Provides essential information on all aspects of multilayer films in flexible packaging including processing properties materials and end use Bridges the gap between scientific principles and practical challenges Includes explanations to assist practitioners in overcoming challenges Enables the reader to address new challenges such as design for sustainability and eCommerce

**Subject Guide to Books in Print**, 1991

**Physics Briefs**, 1993

**Statistical Physics of Polymers** Toshihiro Kawakatsu, 2013-03-09 This book is an introductory textbook on the statistical mechanics of polymers and complex fluids aimed at senior undergraduate and graduate students and non specialist researchers who are starting research in this field Modern statistical mechanics on polymers and complex fluids is based on many fields such as chemical physics statistical mechanics quantum mechanics stochastic processes theory of phase transitions hydrodynamics rheology and so on This book provides an overview of the basic concepts and methods used in current research on the physics of polymers and complex fluids Using simple but essential examples we describe how to derive the physical properties of polymers theoretically focusing on the structure and dynamics on mesoscopic scales Here

the term mesoscopic scales means intermediate lengths and time scales between the microscopic atomic scale and the macroscopic scale Properties on mesoscopic scales are the central issue of the physics of polymers and complex fluids because these materials are well characterized by spatiotemporal structures on these scales where we can extract universal properties that are independent of the microscopic details of the system

**Contributions to Science**, 2001 **Polymer Mechanochemistry** Roman Boulatov, 2015-10-17 The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology medicine and materials science The goal of each thematic volume is to give the non specialist reader whether in academia or industry a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole The most significant developments of the last 5 to 10 years are presented using selected examples to illustrate the principles discussed The coverage is not intended to be an exhaustive summary of the field or include large quantities of data but should rather be conceptual concentrating on the methodological thinking that will allow the non specialist reader to understand the information presented Contributions also offer an outlook on potential future developments in the field Review articles for the individual volumes are invited by the volume editors Readership research chemists at universities or in industry graduate students

Fundamental Polymer Science Ulf W. Gedde, Mikael S. Hedenqvist, 2019-12-20 This successor to the popular textbook Polymer Physics Springer 1999 is the result of a quarter century of teaching experience as well as critical comments from specialists in the various sub fields resulting in better explanations and more complete coverage of key topics With a new chapter on polymer synthesis the perspective has been broadened significantly to encompass polymer science rather than just polymer physics Polysaccharides and proteins are included in essentially all chapters while polyelectrolytes are new to the second edition Cheap computing power has greatly expanded the role of simulation and modeling in the past two decades which is reflected in many of the chapters Additional problems and carefully prepared graphics aid in understanding Two principles are key to the textbook's appeal 1 Students learn that independent of the origin of the polymer synthetic or native the same general laws apply and 2 students should benefit from the book without an extensive knowledge of mathematics Taking the reader from the basics to an advanced level of understanding the text meets the needs of a wide range of students in chemistry physics materials science biotechnology and civil engineering and is suitable for both masters and doctoral level students Praise for the previous edition an excellent book well written authoritative clear and concise and copiously illustrated with appropriate line drawings graphs and tables Polymer International an extremely useful book It is a pleasure to recommend it to physical chemists and materials scientists as well as physicists interested in the properties of polymeric materials Polymer News This valuable book is ideal for those who wish to get a brief background in polymer science as well as for those who seek a further

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## **Table of Contents Flexible Polymer Chains In Elongational Flow Theory And Experiments**

1. Understanding the eBook Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - The Rise of Digital Reading Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Advantages of eBooks Over Traditional Books
2. Identifying Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - User-Friendly Interface
4. Exploring eBook Recommendations from Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Personalized Recommendations
  - Flexible Polymer Chains In Elongational Flow Theory And Experiments User Reviews and Ratings
  - Flexible Polymer Chains In Elongational Flow Theory And Experiments and Bestseller Lists

5. Accessing Flexible Polymer Chains In Elongational Flow Theory And Experiments Free and Paid eBooks
  - Flexible Polymer Chains In Elongational Flow Theory And Experiments Public Domain eBooks
  - Flexible Polymer Chains In Elongational Flow Theory And Experiments eBook Subscription Services
  - Flexible Polymer Chains In Elongational Flow Theory And Experiments Budget-Friendly Options
6. Navigating Flexible Polymer Chains In Elongational Flow Theory And Experiments eBook Formats
  - ePub, PDF, MOBI, and More
  - Flexible Polymer Chains In Elongational Flow Theory And Experiments Compatibility with Devices
  - Flexible Polymer Chains In Elongational Flow Theory And Experiments Enhanced eBook Features
7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Highlighting and Note-Taking Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Interactive Elements Flexible Polymer Chains In Elongational Flow Theory And Experiments
8. Staying Engaged with Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Flexible Polymer Chains In Elongational Flow Theory And Experiments
9. Balancing eBooks and Physical Books Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Flexible Polymer Chains In Elongational Flow Theory And Experiments
10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
11. Cultivating a Reading Routine Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Setting Reading Goals Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Fact-Checking eBook Content of Flexible Polymer Chains In Elongational Flow Theory And Experiments
  - Distinguishing Credible Sources
13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
- Exploring Educational eBooks

### 14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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