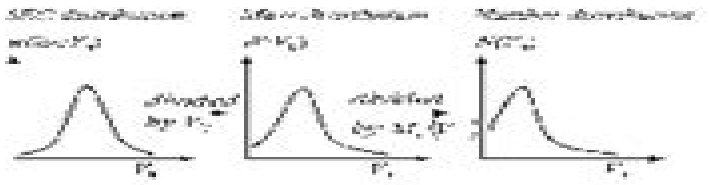
Macromolecular Theory and Simulations

Theory of Multiple-Detection Size-Exclusion Chromatography of Complex Branched Polymers

Marianne Gaborieau, Robert G. Gilbert, Angus Gray-Weale, Javier M. Hernandez, Patrice Castignolles*

SEC separates complex branched polymers by hydrodynamic volume, rather than by molecular weight or branching characteristics. Equations relating the response of different types of detectors are derived including band broadening, by defining a distribution function $N'(M,V_h)$, the number of chains with molecular weight M and hydrodynamic volume V_h. While the true molecular weight distribution of complex polymers cannot be determined by SEC, irrespective of the detector used, the formalism enables multiple detection SEC data to be processed to both analyze the polymer sample and reveal mechanistic information about polymer synthesis. The formalism also shows how the true weight- and number-average molecular weight, $\overline{M}_w$ and $\overline{M}_n$, can be obtained from correct processing of the hydrodynamic volume distributions.



Introduction

Size exclusion chromatography (SEC) is a major technique for analyzing synthetic and natural polymers.[1,2] Benoit[3,4] and others[5–7] have provided evidence that SEC separation occurs by the product of $[\eta] \times M$, where $[\eta]$ is the intrinsic viscosity and M the molecular weight (MW), and not according to MW only. Zimm et al. demonstrated that the presence of long-chain branches significantly changes the hydrodynamic volume at a given MW.[8,9] While for linear polymers there exists a one-to-one relation between MW and the elution time by neglecting band broadening (the conventional calibration curve), this is not the case for complex branched polymers: a sample wherein all chains have the same hydrodynamic volume may have a distribution of molecular weights.[9,10–12] Complex branched polymers not only have a distribution of MWs but also a distribution of chain branch lengths and topologies. They are different from regular branched polymers like regular stars or combs. Complex branched polymers are present in several important families of polymers: (i) dendritic polymers, both biopolymers (e.g., amylopectin[13,14]) and synthetic polymers[15,16] and (ii) statistically (or randomly) branched polymers[17] such as

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Multiple Detection In Size Exclusion Chromatography

André M. Striegel

Multiple Detection In Size Exclusion Chromatography:

Multiple Detection in Size-exclusion Chromatography André M. Striegel,2005 For four decades size exclusion chromatography has played a prominent role in characterizing polymers by determining the polymer s molar mass averages often not absolutely but relative to some calibration standard Not satisfied scientists now want to determine the absolute molar mass averages and distribution and to characterize their long chain and short chain branching tacticity copolymer and base pair sequences and other matters Oh yes and they want all this as a continuous function of the molar mass of the analyte Fortunately the technique is endowed with a number of detection methods and the 18 papers here explain the role of those various detection methods and the synergistic effect of combining them in different configurations to obtain desired results Distributed in the US by Oxford University Press Annotation 2004 Book News Inc Portland OR booknews com

Multidimensional HPLC of Polymers Harald Pasch,Bernd Trathnigg,2013-06-12 This book presents the principle ideas of combining different analytical techniques in multi dimensional analysis schemes It reviews the basic principles and instrumentation of multi dimensional chromatography and the hyphenation of liquid chromatography with selective spectroscopic detectors and presents experimental protocols for the analysis of complex polymers It is the consequent continuation of HPLC of Polymers from 1999 by the same authors Like its predecessor this book discusses the theoretical background equipment experimental procedures and applications for each separation technique but in contrast treats multi dimensional and coupled techniques Multidimensional HPLC of Polymers intends to review the state of the art in polymer chromatography and to summarize the developments in the field during the last 15 years With its tutorial and laboratory manual style it is written for beginners as well as for experienced chromatographers and will enable its readers polymer chemists physicists and material scientists as well as students of polymer and analytical sciences to optimize the experimental conditions for their specific separation problems **Polymer Science: A Comprehensive Reference** ,2012-12-05 The progress in polymer science is revealed in the chapters of Polymer Science A Comprehensive Reference Ten Volume Set In Volume 1 this is reflected in the improved understanding of the properties of polymers in solution in bulk and in confined situations such as in thin films Volume 2 addresses new characterization techniques such as high resolution optical microscopy scanning probe microscopy and other procedures for surface and interface characterization Volume 3 presents the great progress achieved in precise synthetic polymerization techniques for vinyl monomers to control macromolecular architecture the development of metallocene and post metallocene catalysis for olefin polymerization new ionic polymerization procedures and atom transfer radical polymerization nitroxide mediated polymerization and reversible addition fragmentation chain transfer systems as the most often used controlled living radical polymerization methods Volume 4 is devoted to kinetics mechanisms and applications of ring opening polymerization of heterocyclic monomers and cycloolefins ROMP as well as to various less common polymerization techniques Polycondensation and non chain

polymerizations including dendrimer synthesis and various click procedures are covered in Volume 5 Volume 6 focuses on several aspects of controlled macromolecular architectures and soft nano objects including hybrids and bioconjugates Many of the achievements would have not been possible without new characterization techniques like AFM that allowed direct imaging of single molecules and nano objects with a precision available only recently An entirely new aspect in polymer science is based on the combination of bottom up methods such as polymer synthesis and molecularly programmed self assembly with top down structuring such as lithography and surface templating as presented in Volume 7 It encompasses polymer and nanoparticle assembly in bulk and under confined conditions or influenced by an external field including thin films inorganic organic hybrids or nanofibers Volume 8 expands these concepts focusing on applications in advanced technologies e g in electronic industry and centers on combination with top down approach and functional properties like conductivity Another type of functionality that is of rapidly increasing importance in polymer science is introduced in volume 9 It deals with various aspects of polymers in biology and medicine including the response of living cells and tissue to the contact with biofunctional particles and surfaces The last volume is devoted to the scope and potential provided by environmentally benign and green polymers as well as energy related polymers They discuss new technologies needed for a sustainable economy in our world of limited resources Provides broad and in depth coverage of all aspects of polymer science from synthesis polymerization properties and characterization methods and techniques to nanostructures sustainability and energy and biomedical uses of polymers Provides a definitive source for those entering or researching in this area by integrating the multidisciplinary aspects of the science into one unique up to date reference work Electronic version has complete cross referencing and multi media components Volume editors are world experts in their field including a Nobel Prize winner *Macromolecular Separation Science* André M. Striegel,2025-06-04 This book provides a comprehensive guide to macromolecular separation science It is unique in its in depth combined coverage of the fundamentals and applications of each individual technique This includes both widely employed as well as niche methods It is also comprehensive regarding the instrumentation especially but not limited to detectors employed as well as the physical and chemical information obtained from various separations detector couplings and also from multi dimensional separations Abundant figures and tables combine to illustrate each point This book provides an indispensable guide for those working in the field of macromolecular separation science to those seeking information about individual techniques to polymer scientists and chromatographers in general and to students beginning practitioners and experts alike **Biophysical Characterization of Proteins in Developing Biopharmaceuticals** Damian J. Houde,Steven A. Berkowitz,2014-09-05 Biophysical Characterization of Proteins in Developing Biopharmaceuticals is concerned with the analysis and characterization of the higher order structure HOS or conformation of protein based drugs Starting from the very basics of protein structure this book takes the reader on a journey on how to best achieve this goal using the key relevant and

practical methods commonly employed in the biopharmaceutical industry today as well as up and coming promising methods that are now gaining increasing attention As a general resource guide this book has been written with the intent to help today s industrial scientists working in the biopharmaceutical industry or the scientists of tomorrow who are planning a career in this industry on how to successfully implement these biophysical methodologies In so doing a keen focus is placed on understanding the capability of these methodologies in terms of what information they can deliver Aspects of how to best acquire this biophysical information on these very complex drug molecules while avoiding potential pitfalls in order to make concise well informed productive decisions about their development are key points that are also covered Presents the reader with a clear understanding of the real world issues and challenges in using these methods Highlights the capabilities and limitations of each method Discusses how to best analyze the data generated from these methods Points out what one needs to look for to avoid making faulty conclusions and mistakes In total it provides a check list or road map that empowers the industrial scientists as to what they need to be concerned with in order to effectively do their part in successfully developing these new drugs in an efficient and cost effective manner Nanomaterials in Chromatography Chaudhery Mustansar Hussain,2018-06-08 Nanomaterials in Chromatography Current Trends in Chromatographic Research Technology and Techniques provides recent advancements in the wide variety of chromatographic techniques applied to nanotechnology As nanomaterials unique properties can improve detection sensitivity and miniaturize the devices used in analytical procedures they can substantially affect the evaluation and analysis ability of scientists and researchers and foster exciting developments in separation science The book includes chapters on such crucial topics as the use of nanomaterials in sample preparation and the legalization of nanomaterials along with a section on reducing the cost of the analysis process both in terms of chemicals and time consumption Presents several techniques for nanomaterials in chromatography including well known materials like carbon nanomaterials and functionalized nanomaterials Includes suggested readings at the end of each chapter for those who need further information or specific details from standard handbooks to journal articles Covers not only applications of nanomaterials in chromatography but also their environmental impact in terms of toxicity and economic effects **Advances in Physicochemical Properties of Biopolymers (Part 1)** Martin Masuelli,Denis Renard,2017-07-05 The last two decades have seen a number of significant advances in the methodology for evaluating the molecular weight distributions of polydispersed macromolecular systems in solution at the molecular level This reference presents reviews on the progress in different analytical and characterization methods of biopolymers Readers will find useful information about combinations of complex biopolymer analysis such as chromatographic or membrane based fractionation procedures combined with multiple detectors on line multi angle laser light scattering or MALLS Key topics include refractive index UV Vis absorbance and intrinsic viscosity detection systems advances in SEC MALLS size exclusion chromatography coupled to multi angle laser light scattering and FFF MALLS field flow fractionation coupled on line to MALLS HPSEC A4F MALLS

matrix assisted laser desorption ionization MALDI electrospray ionization ESI mass spectrometry nuclear magnetic resonance NMR spectroscopy This reference is intended for students of applied chemistry and biochemistry who require information about biopolymer analysis and characterization **Monitoring Polymerization Reactions** Wayne F. Reed,Alina M. Alb,2014-01-21 Offers new strategies to optimize polymer reactions With contributions from leading macromolecular scientists and engineers this book provides a practical guide to polymerization monitoring It enables laboratory researchers to optimize polymer reactions by providing them with a better understanding of the underlying reaction kinetics and mechanisms Moreover it opens the door to improved industrial scale reactions including enhanced product quality and reduced harmful emissions Monitoring Polymerization Reactions begins with a review of the basic elements of polymer reactions and their kinetics including an overview of stimuli responsive polymers Next it explains why certain polymer and reaction characteristics need to be monitored The book then explores a variety of practical topics including Principles and applications of important polymer characterization tools such as light scattering gel permeation chromatography calorimetry rheology and spectroscopy Automatic continuous online monitoring of polymerization ACOMP reactions a flexible platform that enables characterization tools to be employed simultaneously during reactions in order to obtain a complete record of multiple reaction features Modeling of polymerization reactions and numerical approaches Applications that optimize the manufacture of industrially important polymers Throughout the book the authors provide step by step strategies for implementation In addition ample use of case studies helps readers understand the benefits of various monitoring strategies and approaches enabling them to choose the best one to match their needs As new stimuli responsive and intelligent polymers continue to be developed the ability to monitor reactions will become increasingly important With this book as their guide polymer scientists and engineers can take full advantage of the latest monitoring strategies to optimize reactions in both the lab and the manufacturing plant **Size Exclusion Chromatography** Theodore Provder,1984 JIRCAS Working Report ,2012 **JIRCAS** □□□□□□□□ ,2012-03 **Starch in Food** Lars Nilsson,2024-05-15 Starch in Food Structure Function and Applications Third Edition is now fully updated with eleven new chapters covering hot areas for starch applications such as starch based pickering emulsifiers starch for structuring gluten free bread products and starch microspheres for encapsulation of probiotic bacteria Sections illustrate how plant starch can be analyzed and modified including chapters on analysis of starch molecular structure molar mass and size the relationship between structure and digestion of starch sources of starch including new chapters on cereal root and tuber and pulse starches and starch applications with a new chapter on utilizing starches in product development in baked products and in gluten free bread Starch selection is one of the most complex areas for a product developer yet starch is key to solving formulation challenges when developing products to meet many of the emerging consumer trends This book aids the end user on acquiring knowledge on fundamental starch aspects such as granular and molecular structure and properties

analysis biosynthesis and general functionality of starch in foods Thoroughly revised edition bringing updated and new chapters covering the fundamentals of starch applications Explores starch aspects such as granular and molecular structure and properties analysis biosynthesis and general functionality of starch in foods Offers insight into how starch related formulation challenges can be addressed *Practical High-Performance Liquid Chromatography* Veronika Meyer,1994-04-12 Updated and improved this edition discusses both practical and theoretical aspects along with the possibilities and problems associated with HPLC Reflects numerous new details and recent advancements in HPLC techniques Offers the latest information on current chromatographic practice and covers equipment preparation column packing and regeneration commercially available stationary phases and much more **Analysis of Polymers** ,1992 Biomass Sugimoto Tomoko,Cheu Peng Leh,2012 *Polymer Biocatalysis and Biomaterials* American Chemical Society. Meeting,2005 Likewise biomaterials comprise an equally exciting field of research that finds many applications in dental surgical and medical areas Both fields are highly interdisciplinary requiring at various times knowledge and expertise in organic and polymer chemistry material science biochemistry molecular biology and chemical engineering Engineered Materials Abstracts ,1995-10 *Journal of Chromatography* ,2002 **Papers Presented at the ... Meeting** American Chemical Society. Division of Polymer Chemistry,1996 **American Book Publishing Record** ,2005

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