Current Employer: Oak Ridge National Laboratory
Bldg: 8610 Rm: M-372 MS: 6494
9500 Spallation Drive
Oak Ridge, TN 37830

Phone: 865-341-1269
Fax: 865-574-1753
Email: arnouldma@ornl.gov
Employer Page: https://www.ornl.gov/staff-profile/mark-arnould
Orcid ID: https://orcid.org/0000-0003-0172-8311
Google Scholar: https://scholar.google.com/citations?user=jVskMwYAAAAJ&hl=en

Mark A. Arnould

Current Research

Application of MALDI-TOF mass spectrometric techniques coupled with GPC in solving novel synthetic polymer/materials research problems including structural determination, sequencing, minor component analysis and quantitation. MALDI-ToF MS imaging of biological samples.

Education

Aug. 1998 - May 2003 University of Akron Akron, OH
- **Ph.D.**, Chemistry
- Dissertation title: Mass Spectrometric Studies of Synthetic Polymers.

Sept. 1992 - May 1998 University of Akron Akron, OH
- **B.S.**, Chemistry
- Two years of undergraduate research in free-radical polymerization in the lab of Dr. H. James Harwood.

Experience

Apr. 2019 - now Oak Ridge National Lab Oak Ridge, TN
Macromolecular Nanomaterials
Center for Nanophase Materials Sciences
Physical Sciences Directorate
Group Leader: Rigoberto Advincula
- MALDI-TOF MS
- GPC
- Develop/expand MALDI-TOF MS program for the analysis of synthetic materials
  - Develop methods
  - Perform all MALDI-ToF Analyses
  - Work with users and expand user base
  - See current research interests
- MALDI-ToF MS imaging of biological Samples
  - Tissue
  - Other organic materials

Feb. 2005 - Apr. 2019 XEROX CORPORATION Webster, NY
Analytical Services
Group Leader: Robin L. Sheppard
- MALDI-TOF MS and Analytical Chemistry (emphasis on GPC)
- Develop MALDI-TOF MS program for the analysis of synthetic materials used in toner and other Xerox products (raw materials).
  - Purchase MALDI-ToF mass spectrometer
  - Set up laboratory
  - Develop methods
  - Perform all MALDI-ToF Analyses
- MALDI-TOF MS analysis of Xerox products

- Developed and perform GPC-MALDI MS
- TLC-MALDI-ToF
- Surface MALDI-ToF
- See current research interests

- GPC
  - Supervise GPC lab
  - Xerox GPC Referee lab
  - Perform all GPC testing in Analytical Services (back-up on HT-GPC)
  - Redeveloped and modernized high speed GPC methods, equipment and column
  - Standardized high speed GPC methods and equipment across sites
  - Maintain all GPC equipment in Analytical Services (except HT-GPC)
  - Experience with UV, RI and Triple Detector (RI, Viscometry and Light Scattering)
  - Developed methods and perform all Triple Detector testing and maintain equipment
  - Preparative GPC and Fraction Collection
  - High-temperature GPC analysis
- Orbitrap high resolution mass spectrometry
  - Single component and mixture analysis
  - Polymer extract analysis
- GC-MS
  - Quantitation
  - Monomer ID
  - Pyrolysis

Jul. 2003 - Feb. 2005 NIST Gaithersburg, MD
Polymers Division
National Research Council Post-Doctoral Fellow
Project Leader: William E. Wallace
- MALDI-TOF MS
- Interest included:
  - The application of novel MALDI-TOF instrumentation
  - Chemical modification of synthetic polymers for covalent cationization
  - Understanding the MALDI process using novel instrumentation
  - The gas-phase ionization of polymer molecules using transition metal complexes

Aug. 1998 - May 2003 University of Akron Akron, OH
Graduate Researcher
Advisor: Professor Chrys Wesdemiotis
- MALDI-TOF MS
- UCB MS research assistantship Aug. 2001 - Dec. 2002,
- Mass spectrometry research assistantship Dec. 2000 - Aug 2001
  - Polyester analysis (MALDI and ESI) for UCB Chemicals Co
  - Polymer analysis (anionic, cationic and condensation)
  - Analyze all samples for the polymer science department

Dec. 2002 - May 2003 University of Akron Akron, OH
Aug. 1998 - Dec. 2000
Teaching Assistant
- General and Organic Biochemistry Laboratory I
- Principles of Chemistry Laboratories I and II
- Qualitative Analysis Laboratory
- Organic Chemistry Laboratory I
- Advanced Chemistry Laboratory IV
  - Taught introductory lectures for each session
  - Instructed students on the operation of the required instrumentation

Awards

- Undergraduate Analytical Chemist Award, Chemistry Department, May 1998
- B.F. Goodrich Research Award, Chemistry Department, May 2000
- D'Ianni Fellowship, Chemistry Department, 1998-2000
- ASMS Travel Award, 49th ASMS Conference, May 27-31, 2001, Chicago, IL
- National Research Council post-doctoral fellowship at the National Institute of Standards and Technology

Professional Societies

- The American Society for Mass Spectrometry
- The American Chemical Society

References

Dr. Rigoberto Advincula
Oak Ridge National Lab
Bldg: 8610 Rm: M-362 MS: 6494
9500 Spallation Drive
Oak Ridge, TN 37830
865-241-9060

Dr. Robin L. Sheppard
XEROX Corporation
800 Phillips Road
Mail Stop 139-64A
Webster, NY 14580
585-422-6384

Dr. William E. Wallace
National Institute of Standards and Technology
100 Bureau Drive
M/S 8320
Gaithersburg, MD 20899-8320
301-975-5886

Dr. Chrys Wesdemiotis
Dept. of Chemistry
The University of Akron
190 E. Buchtel Commons
Akron, OH 44325-3601
330-972-7699

Publication and Presentation Lists Attached

Publications:

1 Wesdemiotis, Chrys; Arnould, Mark A.; Lee, Youngjoon; Quirk, Roderic P. **MALDI TOF mass spectrometry of the products from novel anionic polymerizations.** Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (2000), 41(1), 629-630.

2 Wesdemiotis, Chrys; Arnould, Mark A.; Lee, Youngjoon; Quirk, Roderic P. **MALDI-TOF mass spectrometry of the products from novel anionic polymerizations.** Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, 2000 (2000), POLY-018.

3 Quirk, Roderic P.; Ge, Qing; Arnould, Mark A.; Wesdemiotis, Chrys. **Functionalization of poly(styryllithium) with 1-butene oxide.** Macromolecular Chemistry and Physics (2001), 202(9), 1761-1767.

4 Arnould, M. A.; Wesdemiotis, C.; Geiger, R. J.; Park, M. E.; Buehner, R. W. **Structural characterization of polyester copolymers by MALDI mass spectrometry.** Athens Conference on Coatings: Science and Technology, Proceedings, 27th, Athens, Greece, July 2-6, 2001 (2001), 399-410.

5 Quirk, Roderic P.; Mathers, Robert T.; Wesdemiotis, Chrys; Arnould, Mark A.. **Investigation of Ethylene Oxide Oligomerization during Functionalization of Poly(styryl)lithium Using MALDI-TOF MS and NMR.** Macromolecules (2002), 35(8), 2912-2918.

6 Quirk, Roderic P.; Gomochak, Deanna L.; Wesdemiotis, Chrys; Arnould, Mark A.. **Synthesis of diene-functionalized macromonomers via functionalization of polymeric organolithiums with 3,4-epoxy-1-butene.** PMSE Preprints (2002), 87, 160-161.

7 Quirk, Roderic P.; Mathers, Robert T.; Ma, Jing-Jing; Wesdemiotis, Chrys; Arnould, Mark A.. **Reaction of polymeric organolithium compounds with ethylene oxide in hydrocarbon solution: determination of extent of oligomerization.** Macromolecular Symposia (2002), 183(IUPAC International Symposium on Ionic Polymerization, 2001), 17-22.

8 Arnould, Mark A.; Wesdemiotis, Chrys; Geiger, Robert J.; Park, Michael E.; Buehner, Rita W.; Vanderorst, Daniel. **Structural characterization of polyester copolymers by MALDI mass spectrometry.** Progress in Organic Coatings (2002), 45(2-3), 305-312.

9 Quirk, Roderic P.; Gomochak, Deanna L.; Wesdemiotis, Chrys; Arnould, Mark A.. **Synthesis of diene-functionalized macromonomers via functionalization of polymeric organolithiums with 3,4-epoxy-1-butene.** Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002), PMSE-002.

10 Wesdemiotis, Chrys; Arnould, Mark A.; Quirk, Roderic P. **End group characterization in anionic polymerizations via mass spectrometry methods.** Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), PMSE-079.

11 Quirk, R. P.; Guo, Ya; Wesdemiotis, Chrys; Arnould, Mark A.. **Functionalization of polymeric organolithium compounds with formaldehyde.** Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), PMSE-313.

12 Quirk, Roderic P.; Gomochak, Deanna L.; Wesdemiotis, Chrys; Arnould, Mark A.. **Functionalization of polymeric organolithium compounds with 3,4-epoxy-1-butene: Precursors for diene-functionalized macromonomers.** Journal of Polymer Science, Part A: Polymer Chemistry (2003), 41(7), 947-957.

13 Wesdemiotis, Chrys; Arnould, Mark A.; Gomochak, Deanna L.; Pickel, Joseph M.; Quirk, Roderic P. **End group characterization in anionic polymerizations via mass spectrometry methods.** PMSE Preprints (2003), 88, 130-131.

14 Quirk, Roderic P.; Guo, Ya; Wesdemiotis, Chrys; Arnould, Mark A.. **Functionalization of polymeric organolithium compounds with formaldehyde.** PMSE Preprints (2003), 88, 542-543.

15 Quirk, Roderic P.; Guo, Ya; Wesdemiotis, Chrys; Arnould, Mark A.. **Functionalization of polymeric organolithium compounds with formaldehyde.** Journal of Polymer Science, Part A: Polymer Chemistry (2003), 41(16), 2435-2453.

16 Quirk, Roderic P.; Jiang, Kevin; Yang, Huimin; Arnould, Mark A.; Wesdemiotis, Chrys. **Recent advances in anionic synthesis of chain-end functionalized elastomers.** Rubber Expo 2001, Fall Technical Program, 160th, Cleveland, OH, United States, Oct. 16-20, 2001 (2001), 1115-1139.

17 Quirk, Roderic P.; Gomochak, Deanna L.; Bhatia, Rajeev S.; Wesdemiotis, Chrys; Arnould, Mark A.; Wollyung, Kathleen. **Synthesis of diene-functionalized macromonomers via functionalization with hexa-1,3,5-triene.** Macromolecular Chemistry and Physics (2003), 204(18), 2183-2196.

18 Arnould, Mark A.. **Mass Spectrometric Studies of Synthetic Polymers.** (2003), 156 pp.

19 Quirk, Roderic P.; You, Fengxiang; Wesdemiotis, Chrys; Arnould, Mark A.. **Anionic Synthesis and Characterization of ω-Hydroxyl-Functionalized Poly(1,3-cyclohexadiene).** Macromolecules (2004), 37(4), 1234-1242.

20 Quirk, Roderic P.; Guo, Ya; Wesdemiotis, Chrys; Arnould, Mark A.. **Investigation of ethylene oxide oligomerization during functionalization of poly(butadienyl)lithium using MALDI-TOF MS and 1H NMR analyses.** Polymer (2004), 45(10), 3423-3428.

21 Arnould, Mark A.; Polce, Michael J.; Quirk, Roderic P.; Wesdemiotis, Chrys. **Probing chain-end functionalization reactions in living anionic polymerization via matrix-assisted laser desorption ionization time-of-flight mass spectrometry.** International Journal of Mass Spectrometry (2004), 238(3), 245-255.

22 Wallace, W. E.; Arnould, M. A.; Knochenmuss, R. **2,5-Dihydroxybenzoic acid: laser desorption/ionisation as a function of elevated temperature.** International Journal of Mass Spectrometry (2005), 242(1), 13-22.

23 Arnould, Mark A.; Vargas, Rafael; Buehner, Rita W.; Wesdemiotis, Chrys. **Tandem mass spectrometry characteristics of polyester anions and cations formed by electrospray ionization.** European Journal of Mass Spectrometry (2005), 11(2), 243-256.

24 Quirk, Roderic P.; Pickel, Joseph M.; Arnould, Mark A.; Wollyung, Kathleen M.; Wesdemiotis, Chrys. **Efficient Synthesis of ω-(p-Vinylbenzyl)polystyrene by Direct Functionalization of Poly(styryl)lithium with p-Vinylbenzyl Chloride in Hydrocarbon Solvent with Lithium 2,3-Dimethyl-3-pentoxide.** Macromolecules (2006), 39(5), 1681-1692.

25 Quirk, Roderic P.; Kim, Young J.; Gijo, Ya; Wesdemiotis, Chrys; Arnould, Mark A. **Hydroxyl chain-end functionalization of polymeric organolithium compounds with oxetane.** Journal of Polymer Science, Part A: Polymer Chemistry (2006), 44(8), 2684-2693.

26 Wyzgoski, Faith J.; Polce, Michael J.; Wesdemiotis, Chrys; Arnould, Mark A.. **Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry investigations of polystyrene and poly(methyl methacrylate) produced by monoacylphosphine oxide photoinitiation.** Journal of Polymer Science, Part A: Polymer Chemistry (2007), 45(11), 2161-2171.

27 Hong,Wei; Chen, Shaoyun; Sun, Bin; Arnould, Mark A.; Meng, Yuezhong; Yuning Li. **Is a polymer semiconductor having a "perfect" regular structure desirable for organic thin film transistors?** Chemical Science (2015), 6, 3225-3235.

28 Goger, A.; Thompson, M. R.; Pawlak, J. L.; Arnould, M. A.; Klymachyov, A.; Lawton, D. J. W. **Effect of Viscosity on Solvent-Free Extrusion Emulsification: Molecular Structure.** Industrial and Engineering Chemistry Research (2017), 56 (44), 12538–12546.

29 Goger, A.; Thompson, M. R.; Pawlak, J. L.; Arnould, M. A.; Lawton, D. J. W. **Solvent - free polymer emulsification inside a twin−screw extruder.** American Institute of Chemical Engineers Journals (2018), 64, 2113–2123.

30 Goger, A.; Thompson, M. R.; Pawlak, J. L.; Arnould, M. A.; Klymachyov, A.; Sheppard, R.; Lawton, D. J. W. **Inline rheological behavior of dispersed water in a polyester matrix with a twin-screw extruder.** Polymer Engineering and Science (2018), 58, 775-783.

31 Goger, A.; Thompson, M. R.; Pawlak, J. L.; Arnould, M. A.; Lawton, D. J. W. **Effect of Viscosity on Solvent-Free Extrusion Emulsification: Varying System Temperature.** Industrial and Engineering Chemistry Research (2018), 57 (36), 12071–12077.

Conference Presentations:

31st Central Regional ACS Meeting, June 21-23, 1999 Columbus, OH.
Talk: *Arnould, M. A.; Wesdemiotis, C.; Lee, y.; Quirk, R. P. MALDI-TOF Mass Spectrometric Analysis of Anionically Prepared Polystyrenes.

1999 Ontario Gas Phase Ion Chemists' Meeting, Trent University, October 29-30, 1999, Peterborough, Ontario, Canada.
Talk: *Arnould, M. A.; Wesdemiotis, C. Compositional and Structural Analysis of Polymers by MALDI Mass Spectrometry.

219th National ACS Meeting, May 26-31, 2000, San Francisco, CA.
Invited Talk: * Wesdemiotis, C.; Arnould, M. A.; Lee, y.; Quirk, R. P. MALDI-TOF Mass Spectrometry of the Products from Novel Anionic Polymerizations.

48th ASMS Conference, June 10-15, 2000, Long Beach, CA.
Poster: * Arnould, M. A.; Wesdemiotis, C.; Lee, y.; Quirk, R. P. Product Analysis of Novel Anionic Polymerizations by MALDI-TOF MS.

2000 Ontario Gas Phase Ion Chemists' Meeting, Trent University, October 29-30, 1999, Peterborough, Ontario, Canada.
Talk: *Arnould, M. A.; Wesdemiotis, C. Composition and Sequence Characterization of Polyester Copolymers.

49th ASMS Conference, May 27-31, 2001, Chicago, IL.
Talk: * Wesdemiotis, C; Arnould, M. A.; Cheong, T. H.; Quirk, R. P. The Use of Functional and Chain-extended Initiators in the Anionic Polymerization of Dienes.
Talk: *Arnould, M. A.; Wesdemiotis, C. The Application of MALDI-TOF Tandem Mass Spectrometry in the Sequencing of Polyester Monomers.

2001 Athens Conference on coatings: Science and Technology, July 2-6, Vouliagmeni (Athens), Greece.
Talk: *Wesdemiotis, C.; Arnould, M. A.; Geiger, R. J.; Park, M. E.; Buehner, R. W.; Vandervost, D. Structural and Molecular Characterization of Polyesters by MALDI Mass Spectrometry.

18th Southern Ontario Ion Chemistry Conference, August 13-15, 2001, Leslie Frost Center, Ontario, Canada.
Talk: *Arnould, M. A.; Wesdemiotis, C. Characterization of Polybutadienes with Functional End

Groups by MALDI Mass Spectrometry.

50th ASMS Conference, June 6-12, 2002, Orlando, FL.
Talk: * Wesdemiotis, C; Arnould, M. A.; Gomochak, D.; Quirk, R. P. Effect of Chain-end Functionality on Polymer Composition in Living Anionic Polymerizations.
Talk: *Arnould, M. A.; Wesdemiotis, C.; Buehner, R.; Vargas, R. R. Sequence determination of Polyester Copolymers.

224th National ACS Meeting, August 18-22, 2002, Boston, MA.
Talk: *Quirk, R. P.; Gomochak, Deanna, L.; Wesdemiotis, Chrys; Arnould, M. A. Synthesis of Diene-Functionalized Macromonomers via Functionalization of Polymeric Organolithiums with 3,4-epoxy-1-butene.

225th National ACS Meeting, March 23-27, 2003, New Orleans, LA.
Talk: *Wesdemiotis, Chrys; Arnould, M. A.; Quirk, R. P. End Group Characterization in Anionic Polymerizations via Mass Spectrometry Methods.

225th National ACS Meeting, March 23-27, 2003, New Orleans, LA.
Talk: *Quirk, R. P.; Guo, Ya; Wesdemiotis, Chrys; Arnould, M. A. Functionalization of Polymeric Organolithium Compounds with Formaldehyde.

52nd ASMS Conference, May 23-27, 2004, Nashville, TN.
Poster: *Arnould, M. A.; Wallce, W. E.; Knochenmuss, R. Understanding and Optimizing the MALDI Process using a Heated Sample Stage: a 2,5-Dihydroxybenzoic Acid Study.

52nd ASMS Conference, May 23-27, 2004, Nashville, TN.
Poster: *Flynn, K. M.; Wetzel, S. J.; Guttman, C. M.; Arnould, M. A.; Lewis, L. A. MALDI-TOF-MS Characterization of Polycyanoacrylate Generated under Acidic Conditions using “Super Glue” or the Cyanoacrylate Fingerprint Fuming Method.

52nd ASMS Conference, May 23-27, 2004, Nashville, TN.
Poster: *Vakili, Z.; Girard, J. E.; Guttman, C. M.; Arnould, M. A.; Byrd, H.M. Analysis of Covalently Cationized Polystyrenes using Liquid Chromatography and Mass Spectrometry.

54th ASMS Conference, May 28-June 1, 2006, Seattle, WA.
Talk: *Arnould, M. A. and Sheppard, R.L. MALDI-ToF MS and GPC analysis of an Aminium Functionalized Polyester.

55th ASMS Conference, June 3-7, 2007, Indianapolis, IN.
Talk: *Arnould, M. A. Copolymer Analysis using MALDI-ToF Mass Spectrometry and Statistics.

2008 APS March Meeting, Monday–Friday, March 10–14, 2008; New Orleans, LA.
Poster: * Pan, David and Arnould, M.A. MALDI-ToF Analysis of Model Copolymer Blends.

56th ASMS Conference, June 1-5, 2008, Denver, CO.
Polymeric Materials Interest Group Coordinator
Session Chair: Imaging of Polymers/Materials and Surfaces

57th ASMS Conference, May 31-June 4, 2009, Philadelphia, PA.
Polymeric Materials Interest Group Coordinator
Talk: *Arnould, M. A. Polymer Analysis using GPC, Thermospray Deposition and MALDI-ToF Mass Spectrometry.

Society for Applied Spectroscopy – Chicago, Polymer Characterization Workshop, Friday, May 14, 2010, Chicago IL.
Talk: *Arnould, M. A. Industrial Polymer/Material Characterization using MALDI-ToF MS and GPC.

62nd ASMS Conference, June 15-19, 2014, Baltimore, MD.
Poster: Arnould, M. A. Structural and Mixture Characterization of Polysorbate 60 using MALDI-ToF MS, GPC-Spray Deposition and High Resolution MS.

Patents

US 20150044606 - Porous toner and process for making the same - Mang; Mark E., Kmiecik-Lawrynowicz; Grazyna E., Arnould; Mark A., Nguyen; Dieu

US 20190316001 - Release fluid additives - Sambhy, Varun; Badesha, Santokh S.; Klymachyov, Alexander N.; Derleth, David S.; Arnould, Mark A.; Lambie, John R

US 20190317438 - Release fluid for electrostatographic device with amino-containing silicone and nonfunctional silicone to reduce silanol content and improve fixing roller lifetime - Sambhy, Varun; Badesha, Santokh S.; Klymachyov, Alexander N.; Derleth, David S.; Arnould, Mark A.; Lambie, John R.; Quigley, James E.