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Education

1986 Ph.D., Chemical Engineering, Massachusetts Inst. of Tech.; J. B. Howard and J. P. Longwell, advisors.
1974 M.S., Chemical Engineering, Louisiana State University; D. P. Harrison, advisor.
1973 B.S. with High Honors, Chemical Engineering, North Carolina State University.

Professional Employment

2009-present North Carolina State University, Dept of Chemical and Biomolecular Engineering, Professor.
2009-2014 Executive Director, NCSU Institute for Computational Science and Engineering.
2016-2018 Director, Southeast Regional Manufacturing Ctr, Clean Energy Smart Mfg Innovation Institute.
2006-2009 National Science Foundation. Program Director (through Interagency Personnel Agreement) for Combustion, Fire, and Plasma Systems; CBET Cyberinfrastructure programs.
1992-1996 National Institute of Standards and Technology, Gaithersburg MD. Sabbatical IPA Chemical Engineer (1992-93, 1994) and Guest Researcher (1993-1996).
1986-2009 Univ. Massachusetts Amherst, Department of Chemical Engineering. Adjunct Prof (2009-13), Interim Head (2003-2005), Professor (1999-2009), Assoc Prof (1992-99), Asst Prof (1986-92).
1974-1979 Oak Ridge National Laboratory, Coal Technology Program. Research engineer.

Prof. Society Memberships: AIChE (Fellow), American Chemical Society, AAAS, Combustion Institute (Fellow) .

Awards, Honors, and Recognitions

2025 LSU College of Engineering Hall of Distinction.
2023 F.J. & Dorothy Van Antwerpen Award for Service to the Institute, AIChE.
2023 Academy of Chemical Engineers Lectureship, Missouri University of Science and Technology.
2022-2023 Chair, NCSU Research Leadership Academy; 2021-22 Chair-Elect.
2020 Sigma Xi, The Scientific Research Society, NC State University Chapter
2019 NCSU Alumni Association Distinguished Research Awd; NCSU Research Leadership Academy.
2018 Fellow, Combustion Institute.
2017 AIChE Institute Award for Excellence in Industrial Gases Technology.
2015-2016 Leverhulme Trust Distinguished Visiting Professorship, Imperial College, London, UK.
2015 Professeur invité (Visiting Professor), Université de Lorraine, Nancy, France.
2013 Honorary Professor, Nanjing University of Technology.
2010 Philip W. Morrison Jr. Lecturer, Case Western Reserve University.
2009 Director's Award for Collaborative Integration, National Science Foundation (shared).
2008 Gary Leach Award, AIChE (to the Centennial Celebration Organization Committee).
2007 George R. Lappin Award, American Institute of Chemical Engineers.
2006 Outstanding Senior Faculty Award, UMass Amherst College of Engineering.
2005 Fellow, American Institute of Chemical Engineers.
2005 David A. Shirley Award for Outstanding Scientific Achievement, Lawrence Berkeley Natl Lab.
2005 Who's Who among America's Teachers.
2002 William H. Corcoran Award, American Society for Engineering Education.
2001 Materials Science Academic Award, MSI.
2000 *Discovery Magazine* Awards, Top Ten Semifinalist for Technological Innovation.
1996 Magellan 3-Star Web Site Author Award.
1992 Outstanding Junior Faculty Award, UMass Amherst College of Engineering.
1992 BCR / R. A. Glenn Award for Best Paper, A.C.S. Fuel Chemistry Division.
1991 NATE Award (Central New England Section AIChE Tribute to Excellence).
1990-1995 Presidential Young Investigator Award, National Science Foundation.
1990 General Electric Outstanding Teaching Award, UMass Amherst College of Engineering.
1977 National Public Relations Award, American Institute of Chemical Engineers.

Professional Activities

American Institute of Chemical Engineers (AIChE), 2013 President (VP 2012, Past Pres 2014).
Board of Directors, 2008-10. AIChE Foundation, Trustee, 2013-22. Ethics Committee Chair, 2013-18.
Institute Nominating Committee: Chair 2013, 2014; Member 2015, 2022-24. RAPID Board, 2018-23.
BoD Awards Committee Chair, 2014; ED Search Comm, 2021-22; Finance Committee, 2013-14.

Public Affairs and Information Committee (PAIC): Vice Chair 2014-15, Chair 2016-17, Past Chair 2018-19. Chair, Communications Committee, author/editor of "ChE in Context" column in *ChE Progress*, 2017-24.
President's Blue-Ribbon Committee on Government Relations, Chair, 2010-11.
Computational Molecular Science and Engineering Forum. Founding Chair 2000-01, Past Chair 2001-02, Vice Chair for Communications 2002-06.
Exec Bd of the Natl Prog Comm, Member '99-02; 2nd Vice Ch 2003; 1st V-Ch, 2004; Ch, 2005; Past Ch, 2006.
Nanotechnology Science and Engineering Forum. Organizing Comm. 2002; Director member 2002-05.
Catalysis and Reaction Engineering Division, Board member 1999-2002.
Topical Conferences: "Applying Molecular Simulation & Computational Chemistry," Co-chair 1998, 2001.
Central New England Section: Chair 1988-89, Director 1989-92.
Knoxville/Oak Ridge Section: Public Relations Chair 1976, Secretary 1977.

CACHE Corporation (nonprofit organization: Computer Aids for Chemical Engineering):

Board of Trustees 1999-present; Secretary 2000-02; Vice-President 2002-04; President 2004-06.
FOMMS "Fdns of Molecular Modeling and Simulation": Co-Chr 2000; Senior Advisor 2003-09 & 2013-pres.
FOPAM "Foundations of Process/product Analytics and Machine learning", Founding co-chair 2019, 2023.

Combustion Institute, Fellow (2018).

Board of Directors 2002-14, Officer Nominating Committee 2003-04; Board Nom. Comm. 2005, 2018, Chair 2020; Lewis Fellowship Committee 2005-10, Chair 2010; By-Laws Revision Committee, Chair 2010-2013.
Co-Founder, member, and first Chair of the Joint Executive Committee of the U.S. Sections 2001-03.
Colloquium Co-Chair, "Reaction Kinetics of Combustion," 29th Intl. Symp. on Combustion 2001-02; Publications Committee 2000-03; Editorial Committee 1994, 96, 98; Program Subcom. 1989-present.
Eastern States Section (US): Past Chair 2003-05; Chair 2001-03; Vice-Chair 1999-2001; Papers Chair 1997-99; Program Chair 1995-97; Executive Committee member-at-large 1993-99.

Council for Chemical Research: Governing Board 2005-07; Exec. Comm, 2006.

Member, IUPAC Task Group "Selected free radicals and critical intermediates: Thermochemistry," 2000-2014.

Member, DoD High-Performance Computing Challenge Board, 2000-06, 2010-12.

Editorial Advisory Boards, *J. Adv. Mfg. Proc.*, 2018-25; *Int. J. Chem. Kinetics*, 2000-02, *I&EC Res.*, 1998-2000.

Chair, "Applying Molecular and Materials Modeling," Multi-agency international study, 1999-2002.

Consultant: Oak Ridge National Lab (1980), Exxon/M.I.T. Comb Res. Prog. (1986-89), A.D. Little (1994), E.I. DuPont (1999-2002), United Technologies Res. Ctr (2004), American Chemistry Council (2022-23).

LSU Chemical Engineering, Industrial Advisory Board, 2011- present.

North Carolina Museum of Natural Sciences, Governor's Advisory Commission member, 2014-2025.

College and University service (major roles):

NCSU Research Leadership Academy, Vice Chair, 2021-2, Chair, 2022-3.

Research Committee, NCSU College of Engineering, 2009-16.

NCSU OIT, Research Computing Committee, 2013-18; IT Strategic Plan Task Force, NCSU, 2013-14.

UMass Amherst: Tang Lecturer Committee, College of Engineering: Member 2000-01, Chair 2001-06; Univ. Chem Hazards Comm: 1993-99, 2001-02; Publications Bd, Col of Eng, 1994-98.

Departmental service (major assignments): DEI Committee Chair, 2021-24.

Department Head (Interim), Chemical Engineering, University of Massachusetts Amherst, 2003-05.

Faculty Search, NCSU: 2011, Co-chair 2015, 2023; UMass: 1988-9; 1991-2; 1993-4, 2002-3; Chair 2001-2.

Departmental Personnel Committee, UMass: Chair 1993-94, 2001-03; Member 2000-01.

Graduate Program Director, UMass: 1994-97, 2000-01, 2002-03.

Research Interests: Kinetics and reaction engineering

Energy. Molecular-beam mass spectrometry (MBMS) and prediction of elementary-reaction combustion kinetics; modeling with detailed mechanisms. Formation and destruction of small hydrocarbons, biofuels, aromatics, NO_x. Hypergolic materials. Catalysis and catalysts. Analytics and data cyberinfrastructure.

Applied theoretical and computational chemistry. Wavefunction and density-functional calculations to generate thermochemistry of molecules, radicals, and transition states. Reaction theories including Quantum-RRK, RRKM, and Master-Equation theories. Reactive Molecular Dynamics.

Polymer / biopolymer decomposition and flammability. Experiments (TGA, DSC, GCxGC/MS), models.

Teaching Experience

Kinetics and reaction engineering (G,UG), thermodynamics (G), process control (UG), material and energy balances (UG), fluid mechanics (UG), heat transfer (UG), mass transfer (UG), separations (UG), unit-operations laboratory (UG), molecular-scale engineering chemistry (G, G/UG), combustion chemistry (G)

Short courses on computational quantum chemistry with Gaussian, Inc. (1997, 1998), for AIChE (1998, 2001, 2003), for ASEE (2002, 2007, 2017), and for PPEPPD (2007).

Advisor for 29 Ph.D. and 17 M.S. students and 7 post-docs; service on 109 other thesis committees.

Publications: 137, plus five books, 388 presented papers and posters, 30 magazine articles and series blogs.

PHILLIP RAY WESTMORELAND
Extended curriculum vitae
December 6, 2025

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I. HONORS AND AWARDS

Awards, Honors, and Recognitions

2025	Hall of Distinction, LSU College of Engineering.
2023	F.J. & Dorothy Van Antwerpen Award for Service to the Institute, AIChE.
2023	Academy of Chemical Engineers Lectureship, Missouri University of Science and Technology.
2020	Sigma Xi, The Scientific Research Society, NC State University Chapter; Inducted July 2020.
2019	NCSU Alumni Association Outstanding Research Award.
2019	Member, NCSU Research Leadership Academy (2022-23 Chair, 2021-22 Chair-Elect)
2018	Fellow, Combustion Institute.
2017	AIChE Institute Award for Excellence in Industrial Gases Technology.
2015-2016	Leverhulme Trust Visiting Professorship, Imperial College, London, UK.
2015	Professeur invité (Visiting Professor), Université de Lorraine, Nancy, France.
2013	Honorary Professor, Nanjing University of Technology.
2010	Phillip Morrison Lecturer, Case Western Reserve University.
2009	Director's Award for Collaborative Integration, National Science Foundation (shared for Cyber-enabled Discovery and Innovation).
2008	Gary Leach Award, American Institute of Chemical Engineers (to the Centennial Celebration Organization Committee).
2007	George R. Lappin Award, American Institute of Chemical Engineers.
2006	Outstanding Senior Faculty Award, UMass Amherst College of Engineering.
2005	Fellow, American Institute of Chemical Engineers.
2005	David A. Shirley Award for Outstanding Scientific Achievement, Lawrence Berkeley National Laboratory.
2005	Who's Who among America's Teachers.
2002	William H. Corcoran Award, American Society for Engineering Education.
2001	Materials Science Academic Award, MSI.
2000	<i>Discovery Magazine</i> Awards, Top Ten Semifinalist for Technological Innovation.
1996	Magellan 3-Star Web Site Author Award.
1992	Outstanding Junior Faculty Award, UMass Amherst College of Engineering.
1992	BCR / R. A. Glenn Award for Best Paper, A.C.S. Fuel Chemistry Division.
1991	NATE Award (Central <u>N</u> ew England Section <u>A</u> IChE <u>T</u> ribute to <u>E</u> xcellence).
1990-95	Presidential Young Investigator Award, National Science Foundation.
1990	General Electric Outstanding Teaching Award, UMass Amherst College of Engineering.
1977	Public Relations Award, American Institute of Chemical Engineers.

II. RESEARCH ACTIVITIES

II.A. Books (5)

- P.R. Westmoreland, P.A. Kollman, A.M. Chaka, P.T. Cummings, K. Morokuma, M. Neurock, E.B. Stechel, and P. Vashishta. *Applying Molecular and Materials Modeling: An International Comparative Study*, Kluwer Academic, Amsterdam (2002). 430 pages. ISBN No. 1-4020-0906-2.
http://www.wtec.org/loyola/molmodel/mm_final.pdf; <http://books.google.com/books?id=y7OI0ggtzcEC>
- P.R. Westmoreland and G.S. Heffelfinger (eds.). *Applying Molecular Simulations and Computational Chemistry*. AIChE, New York (2001); AIChE Publication No. 147, ISBN No. 0-8169-9759-4.
- P.T. Cummings, P.R. Westmoreland, and Brice Carnahan (eds.). *Foundations of Molecular Modeling and Simulations*, AIChE Symposium Series No. 325, Volume 97 (2001). 328 pages. ISBN No. 0-8169-0839-7.
- Kenneth A. Cox, Peter T. Cummings, Phillip R. Westmoreland (eds.). *Applying Molecular Modeling and Computational Chemistry*. AIChE, New York (1998). 534 pages. ISBN No. 0-8169-9857-4.
- T.J. Mountziaris, G. Paz-Pujalt, F.T.J. Smith, P.R. Westmoreland (eds.). *Gas-Phase and Surface Chemistry in Electronic Materials Processing*, Materials Research Society, Pittsburgh (1994). 556 pages. ISBN No. 1-55899-233-2.

II.B. Papers and chapters (140)

140. H. Ram, P.R. Westmoreland, "Finding Mechanisms and Conditions for Pyrolysis of Perfluorooctanoic Acid (PFOA) Using a Detailed Kinetic Model," *I&EC Research* (Accepted; in proofs).
139. T.J. Mallo, A. Dumas, P.R. Westmoreland, "Molecularly based lumped models of polymer pyrolysis for poly(methyl methacrylate) and polyoxymethylene," *Proc. Combustion Inst.* **41** (2025) 105807. <<https://doi.org/10.1016/j.proci.2025.105807>>
138. H. Ram, T.P. Sadej, C.C. Murphy, T.J. Mallo, P.R. Westmoreland, "Correction to Thermochemistry of Species in Gas-Phase Thermal Oxidation of C₂ to C₈ Perfluorinated Carboxylic Acids," *J. Phys. Chem. A* **129**:13 (2025) 3176–3182. <<https://pubs.acs.org/doi/10.1021/acs.jpca.5c01422>>; published 3/19/2025
137. H. Ram, C. Murphy DePompa, P.R. Westmoreland, "Correction to Thermochemistry of Species in Gas-Phase Thermal Oxidation of C₂ to C₈ Perfluorinated Sulfonic Acids with Extrapolation to C₁₆," *J. Phys. Chem. A* **129**:11 (2025) 2823-2827. <<https://pubs.acs.org/doi/full/10.1021/acs.jpca.5c01423>>
136. R. Cai, K. Yang, X. Wang, M. Rukh, A. S. Bosari, E. Giavedoni, A. Pierce, L. Brody, W. Tang, P. R. Westmoreland, F. Li, "High-throughput design of complex oxides as isothermal, redox-activated CO₂ sorbents for green hydrogen generation," *Energy & Environmental Sci.* **17** (2024) 6279-6290. <<https://doi.org/10.1039/d4ee02119c>>
135. H. Ram, C. Murphy DePompa, P.R. Westmoreland, "Thermochemistry of Species in Gas-Phase Thermal Oxidation of C₂ to C₈ Perfluorinated Sulfonic Acids with Extrapolation to C₁₆," *J. Phys. Chem. A.* **128**:17 (2024) 3387-3395. <<https://doi.org/10.1021/acs.jpca.4c01208>>
134. H. Ram, T.P. Sadej, C.C. Murphy, T.J. Mallo, P.R. Westmoreland, "Thermochemistry of Species in Gas-Phase Thermal Oxidation of C₂ to C₈ Perfluorinated Carboxylic Acids," *J. Phys. Chem. A.* **128**:7 (2024) 1313-1326. <<https://doi.org/10.1021/acs.jpca.3c06937>>
133. M. Grover, P.R. Westmoreland. "Teaching Data Science," *Chem. Eng. Education* **56**:4, 217-218 (2022).
132. Y. Tian, G. Luongo, F. Donat, C. R. Müller, P. R. Westmoreland, F. Li, "Oxygen Non-stoichiometry and Defect Models of Brownmillerite-structured Ca₂MnAlO_{5+δ} for Chemical Looping Air Separation," *ACS Sustainable Chem. & Eng.* **10**:31 (2022) 10393-10402. <https://doi.org/10.1021/acssuschemeng.2c03485>
131. B. Zulueta, S. Tulyani, P. Westmoreland, M. Frisch, E.J. Petersson, G. Petersson, J. Keith, "A Bond-Energy/Bond-Order and Populations Relationship," *J. Chem. Theory Computation* **18**:8 (2022) 4774-4794; online 7/18/2022 at <https://doi.org/10.1021/acs.jctc.2c00334>
130. Y. Tian, P.R. Westmoreland, F. Li, "CaMn_{0.9}Ti_{0.1}O₃ Based Redox Catalysts for Chemical Looping – Oxidative Dehydrogenation of Ethane: Effects of Na₂MoO₄ Promoter and Degree of Reduction on the Reaction Kinetics," *Catalysis Today* (2022); online at <https://doi.org/10.1016/j.cattod.2022.04.026>
129. R.D. Braatz, T.A. Badgwell, P.R. Westmoreland, "Editorial: Foundations in Process Analytics and Machine Learning (FOPAM)," *Computers & Chemical Engineering*, Special Issue: V. Venkatasubramanian (ed.), Article 107225. DOI:10.1016/j.compchemeng.2021.107225
128. J. Clark, P. Thacker, C.J. McGill, J. Miles, P.R. Westmoreland, K. Efimenko, J. Genzer, E. Santiso, "DFT Analysis of Organotin Catalytic Mechanisms in Dehydration Esterification Reactions for Terephthalic Acid and 2,2,4,4-Tetramethyl-1,3-Cyclobutanediol," *J. Phys. Chem. A* **125**:23 (2021) 4943–4956. <https://doi.org/10.1021/acs.jpca.1c00850>
127. C. J. McGill, P. R. Westmoreland, "Molecular Carbonyl Insertion as the Mechanism for Transesterification of Dimethyl Terephthalate with Ethylene Glycol," *Ind. Eng. Chem. Res.* **60**:14 (2021) 5090–5101; <https://doi.org/10.1021/acs.iecr.0c05188>
126. A. Bose, P. R. Westmoreland, "Predicting Electron Ionization Cross-Sections for Organic Molecules using Machine Learning," *J. Phys. Chem. A* **124**:50 (2020) 10600-10615. <https://dx.doi.org/10.1021/acs.jpca.0c06308>
125. V. J. Mascarenhas, C. N. Weber, P. R. Westmoreland, "Estimating Flammability Limits through Predicting Laminar Flame Properties," *Proceedings of the Comb. Institute*, **38**:3 (2021) 4673-4681. <https://doi.org/10.1016/j.proci.2020.06.026>
124. Y. Tian, R. Dudek, P. R. Westmoreland, F. Li, "Effect of Sodium Tungstate Promoter on the Reduction Kinetics of CaMn_{0.9}Fe_{0.1}O₃ for Chemical Looping – Oxidative Dehydrogenation of Ethane," *Chem. Eng. J.* **398** (2020) 125583-124591. <https://doi.org/10.1016/j.cej.2020.125583>
123. Q. Xiong, K. Hong, S. Shu, P. Westmoreland, R. Xiao, "Multiscale numerical simulation of biomass thermochemical conversion: From micro to macro scales," *Fuel Processing Technology* **199** (2020), 106294; <https://doi.org/10.1016/j.fuproc.2019.106294>

122. P.R. Westmoreland, "Pyrolysis Kinetics for Lignocellulosic Biomass-to-Oil from Molecular Modeling," *Current Opinion in Chem. Eng.* **23** (2019) 123–129. <https://doi.org/10.1016/j.coche.2019.03.011> [Invited]
121. C.J. McGill, P.R. Westmoreland, "Monosaccharide Isomer Interconversions Become Significant at High Temperatures," *J. Phys. Chem. A*, **123**:1 (2019) 120–131. doi: 10.1021/acs.jpca.8b07217
120. B. Dlugogorski, J. Al-Nu'airat, X. Gao, N. Zeinali, J. Skut, P. Westmoreland, M. Altarawneh, "Reaction of Phenol with Singlet Oxygen," *Phys. Chem. Chem. Phys.* **21** (2019) 171-183; DOI: 10.1039/c8cp04852e
119. P.R. Westmoreland, C. McCabe, "Revisiting the Future of Chemical Engineering," *Chem. Eng. Prog.* **114**:10 (2018) 26-37.
118. J. Oreluk, C.D. Needham, S. Baskaran, S.M. Sarathy, M.P. Burke, R.H. West, M. Frenklach, P.R. Westmoreland. "Dynamic Chemical Model for H₂/O₂ Combustion Developed through a Community Workflow," arXiv preprint arXiv:1801.10093 (2018).
117. Y. Fenard, A. Gil, G. Vanhove, H.-H. Carstensen, K.M. Van Geem, P.R. Westmoreland, O. Herbinet, F. Battin-Leclerc, "A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants," *Comb. Flame* **191** (2018) 252-269; <https://doi.org/10.1016/j.combustflame.2018.01.006>
115. C.D. Needham, P.R. Westmoreland, "Combustion and Flammability Chemistry for the Refrigerant HFO-1234yf (2,3,3,3-tetrafluoropropene)," *Combustion and Flame* **184** (2017) 176-185; <https://doi.org/10.1016/j.combustflame.2017.06.004>
114. J. Al-Nu'airat, M. Altarawneh, X. Gao, P.R. Westmoreland, B. Z. Dlugogorski, "Reaction of Aniline with Singlet Oxygen (O₂ ¹Δ_g)," *J. Phys. Chem. A* **121** (2017) 3199–3206. <https://doi.org/10.1021/acs.jpca.7b00765>
113. I. Oluwoye, B. Z. Dlugogorski, J. Gore, P. R. Westmoreland, M. Altarawneh, "Enhanced ignition of biomass surrogate in presence of NO_x," *Fire Safety J.* **91** (2017) 235-242. <http://dx.doi.org/10.1016/j.firesaf.2017.03.042>
112. K. Siddique, M. Altarawneh, J. Gore, P.R. Westmoreland, B. Dlugogorski, "Hydrogen Abstraction from Hydrocarbons by NH₂," *J. Phys. Chem. A* **121**:11 (2017) 2221-2231. DOI: 10.1021/acs.jpca.6b12890
111. A. Rodriguez, O. Herbinet, Z. Wang, F. Qi, C. Fittschen, P.R. Westmoreland, F. Battin-Leclerc, "Measuring hydroperoxide chain-branching agents during n-pentane low-temperature oxidation," *Proc. Combust. Inst.* **36** (2017) 333-342. DOI: 10.1016/j.proci.2016.05.044
110. P.R. Westmoreland, P.J. Fahey, "Dehydration and dehydrogenation kinetics of OH groups in biomass pyrolysis," *Chemical Eng. Transactions* **50** (2016) 73-78. DOI: 10.3303/CET1650013.
109. V. Seshadri, P. R. Westmoreland, "Roles of Hydroxyls in the Noncatalytic and Catalyzed Formation of Levoglucosan from Glucose," *Catalysis Today* **269** (2016) 110-121. DOI 10.1016/j.cattod.2015.10.033
108. D. R. Yeates, W. Li, W. Speight, P. R. Westmoreland, T. Russi, A. Packard, M. Frenklach, "Validating and Exploiting Predictive Models by Integrating a Data-Analysis Instrumental Model," *Proc. Combustion Inst.* **35** (2015) 597–605; DOI: 10.1016/j.proci.2014.05.090
107. P. R. Westmoreland, "Opportunities and challenges for a Golden Age of chemical engineering," *Frontiers of Chemical Science and Engineering* **8**(1) (2014) 1-7; <http://link.springer.com/article/10.1007/s11705-014-1416-z>
106. P.R. Westmoreland, "Molecular Kinetics of Making Bio-Oils: Opportunities and Challenges for a Golden Age of Chemical Engineering," *Chemie Ingenieur Technik* **85**:9 (2013) 1357–1360. <https://onlinelibrary.wiley.com/toc/15222640/2013/85/9> [Jahrestagung der Fachgemeinschaft Fluidodynamik und Trenntechnik, Plenarvortrag,]
105. J. Cao, M.A. Meador, M.L. Baba, P.M. Ferreira, M. Madou, W. Scacchi, J.C. Spohrer, C. Teague, P. Westmoreland, X. Zhang, "Chapter 7. Implications: Societal collective outcomes, including manufacturing," in *Convergence of Knowledge, Technology, and Society: Beyond Convergence of Nano-Bio-Info-Cognitive Technologies*, M.C. Roco, W.S. Bainbridge, B. Tonn, G. Whitesides (eds.), (2013) 255-285.
104. S. Li, D. F. Davidson, R. K. Hanson, N. J. Labbe, P. R. Westmoreland, P. Oßwald, K. Kohse-Höinghaus, "Shock Tube Measurements and Model Development for Morpholine Pyrolysis and Oxidation at High Pressures," *Comb. Flame* **160**:9 (2013) 1559-1571. <http://dx.doi.org/10.1016/j.combustflame.2013.03.027>
103. N. J. Labbe, V. Seshadri, T. Kasper, N. Hansen, P. Oßwald, P. R. Westmoreland, "Flame chemistry of tetrahydropyran as a model heteroatomic biofuel," *Proc. Combustion Institute*, **34**:1, (2013) 259–267; DOI: 10.1016/j.proci.2012.07.027

102. V. Seshadri, P. R. Westmoreland, "Concerted reactions and mechanism of glucose pyrolysis and implications for cellulose kinetics," *J. Phys. Chem. A* **116**:49 (2012) 11997-20013. doi: 10.1021/jp3085099. **Cover**
101. N. Hansen, J. A. Miller, S. J. Klippenstein, P. R. Westmoreland, K. Kohse-Höinghaus. "Exploring Formation Pathways of Aromatic Compounds in Laboratory-Based Model Flames of Aliphatic Fuels," *Fizika Goreniya i Vzryva* **48**(5), 17-26, September–October, 2012 / *Combustion, Explosion and Shock Waves (English)* **48**(5), 508-515 (2012).
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II.C. Edited journal issues

- M. Grover, P.R. Westmoreland (editors). Special section on "Teaching Data Science," *Chemical Engineering Education* **56**:4 (2022). (Six papers and editor introduction).
- Q. Xiong, K. Hong, S. Shu, P. Westmoreland, R. Xiao (eds.). Special issue on "Multiscale numerical simulation of biomass thermochemical conversion: From micro to macro scales," *Fuel Processing Technology* **199** (2020), 106294; <https://doi.org/10.1016/j.fuproc.2019.106294>
- P. R. Westmoreland and K. R. Cox, "Computational Chemistry and Its Industrial Applications," *I&EC Research*, **12**, pp. 4149-4221 (1995).
- S. Senkan, A. F. Sarofim, H. R. Semerjian, P. R. Westmoreland (eds.), "Special Issue: Combustion and Incineration in Chemical Engineering," *Combustion Science and Technology*, **82**(1-6), (1992).

II.D. Presentations, posters, and other publications

AIChE Annual Meeting, Boston MA, November 2-6, 2025.

- P385. A. Dumas, T.J. Mallo, P.R. Westmoreland, "Polyoxymethylene-Pyrolysis Models from Experiments and Reactive Molecular Dynamics," Paper 8g.
- P388. M. Manouchehri, P.R. Westmoreland, "Toward Detailed Chemical Mechanisms for the Efficient Destruction of Novichok Neurotoxins," Poster 389e.
- P386. T.J. Mallo, A. Dumas, P.R. Westmoreland, "Molecularly Based Empirical Models for Pyrolysis of Polypropylene and Polyethylene," Paper 584ax.
- P387. P.R. Westmoreland, H. Ram, C.C. Murphy, T.J. Mallo, "Destruction-Reaction Pathways for Perfluorocarboxylic and -Sulfonic Acids from a Detailed Kinetic Model," Paper 635a.
- P384. P.R. Westmoreland, H. Ram, "PFSA Destruction Kinetics Becomes PFCA Destruction Kinetics," International Conference on Chemical Kinetics, Granlibakken, Tahoe City NV, June 8-13, 2025.

US National Combustion Meeting, Boston MA, March 16-19, 2025.

- P383. H. Ram, T.J. Mallo, P.R. Westmoreland, "Flame Mechanisms of Methane/Perfluorinated Carboxylic Acid Blends Inferred Using ncsuPFASmech," Paper 3K09.
- P382. T.J. Mallo, A. Dumas, P.R. Westmoreland, "Molecularly based lumped models of polymer pyrolysis for poly(methyl methacrylate) and polyoxymethylene," Paper 3C05.

AIChE Annual Meeting, San Diego CA, October 27-31, 2024.

- P381. P.R. Westmoreland, C.C. Murphy, H. Ram, T.J. Mallo, J.D. Krug, N. Weber, W. Linak, "Detailed Kinetic Model and Mechanism for Incinerating Perfluorocarboxylic Acids, Perfluorosulfonic Acids, and Their Mixtures," Paper 110b.

- P380. T.J. Mallo, H. Ram, C. Claire Murphy, T.P. Sadej, P.R. Westmoreland, "Predicting Gas-Phase Transport Properties of PFAS for Incineration Models Using Quantum Chemistry, Correlations, and Molecular Simulation," Paper 110f.
- P379. A. Dumas, T.J. Mallo, P.R. Westmoreland, "Developing Reactive Models of Polymer Pyrolysis Using Physical Experiments and Reactive Molecular Dynamics," Paper 672d.
- P378. K. Yang, R. Cai, X. Wang, M. Rukh, A. Saberi Bosari, E. Giavedoni, A. Pierce, L. Brody, W. Tang, P.R. Westmoreland, F. Li, "High-Throughput Design of Phase-Transition CO₂ Sorbents for Green Hydrogen Generation," Paper 48g.
- P377. P.R. Westmoreland, "Chemical Kinetics for Getting Rid of PFAS," NC 2024 PFAS Summit, DoubleTree Hotel RDU, Durham NC, October 17, 2024.
- P376. P.R. Westmoreland, C.C. Murphy, H. Ram, T.J. Mallo, J.D. Krug, N. Weber, W. Linak, "Mechanistic insights into incineration of perfluorocarboxylic and perfluorosulfonic acid mixtures from detailed kinetic modeling." ACS National Meeting, Denver CO, August 18-22, 2024.
- Foundations of Molecular Modeling and Simulation, Snowbird UT, July 28-August 1, 2024.**
- P375. A. Dumas, T.J. Mallo, P.R. Westmoreland, "Capturing Reactions of Polymer Pyrolysis Using Physical Experiments and Reactive Molecular Dynamics," Poster Session.
- P374. T.J. Mallo, C.C. Murphy, H. Ram, P.R. Westmoreland, "Predicting Gas-Phase Transport Properties of PFAS for Incineration Models Using Quantum Chemistry, Correlations, and Molecular Simulation," Poster Session.
- 40th International Symposium on Combustion, Combustion Institute, Milan, Italy, July 21-26, 2024.**
- P373. P.R. Westmoreland, H. Ram, C. Murphy DePompa, T.J. Mallo, J.D. Krug, W.R. Roberson, Nathan Weber, W.P. Linak, "Modeling AFFF/PFAS Incineration Kinetics and Thermochemistry," Work-in-Progress poster 1P089.
- P372. P.R. Westmoreland, C.C. Murphy DePompa, H. Ram, T.J. Mallo, "Predictive Mechanistic Modeling of PFCA Flame Kinetics and Thermochemistry," Flame Chemistry Workshop, FC24.
- P371. P.R. Westmoreland, "New Directions for Chemical Engineering Worldwide," World Digital Congress of Chemical and Biochemical Engineering, 5/21/2024. **[Invited Plenary Lecture.]**
- Eastern States Section of the Combustion Institute, Spring Technical Meeting, March 8-11, 2024, Athens, GA.**
- P370. T.J. Mallo, A. Dumas, P.R. Westmoreland, "Toward molecular mechanisms of poly(methyl methacrylate) pyrolysis," Paper 2B15.
- P369. A. Dumas, T.J. Mallo, P.R. Westmoreland, "Probing mechanisms of polymer pyrolysis in polyoxymethylene homopolymer and copolymer," Paper 2B14.
- P368. H. Ram, T.P. Sadej, C.C. Murphy, T.J. Mallo, P.R. Westmoreland, "Computational thermochemistry for gas-phase thermal oxidation of PFAS components of AFFF," Paper 2B11.
- P367. C.C. Murphy, H. Ram, T.P. Sadej, T.J. Mallo, P.R. Westmoreland, "Comprehensive gas-phase kinetics model and mechanism for the incineration of C₂ to C₈ perfluorinated carboxylic acids," Paper 2B09.
- P366. P.R. Westmoreland, H. Ram, T.P. Sadej, C.C. Murphy, T.J. Mallo, "Development and Application of Detailed Kinetics Mechanisms for PFAS Incineration," AIChE Annual Meeting, Orlando FL, November 5-10, 2023. Paper 659b.
- SERMACS 2023 (Southeast Regional Meeting of the American Chemical Society), Durham NC, October 25-28, 2023.**
- P365. C.C. Murphy, H. Ram, T.P. Sadej, T. Mallo, P.R. Westmoreland, "New ideal-gas thermochemical properties for thermal destruction of C₂ to C₈ perfluorinated carboxylic acids."
- P364. H. Ram, T.P. Sadej, C.C. Murphy, T. Mallo, P.R. Westmoreland, "New gas-kinetics mechanism for thermal destruction of C₂ to C₈ perfluorinated carboxylic acids."
- P363. P.R. Westmoreland, C.C. Murphy, H. Ram, T.P. Sadej, "Chemical mechanisms of incineration for perfluorooctanoic acid," U.S. National Combustion Meeting, Texas A&M University, College Station TX, March 19-22, 2023, Paper 1A03.
- P362. P.R. Westmoreland, H. Ram, T.P. Sadej, C.C. Murphy, "Present Status and New Results for PFAS Destruction Chemistry," AIChE Annual Meeting, Phoenix AZ, November 13-18, 2022, Paper 654g.

- P361. P.R. Westmoreland, H. Ram, T.P. Sadej, C.C. Murphy, "Elementary Reactions for PFAS Destruction Chemistry," 39th International Symposium on Combustion, Vancouver Canada, July 24-29, 2022, Work in Progress Poster 3P052.
- P360. M.J. Haselow, J.S. Haselow, P.R. Westmoreland, "Applying Reactive Molecular Dynamics to Simulate Glucose and Xylose Pyrolysis," Eastern States Section of the Combustion Institute, Spring Technical Meeting, March 6-9, 2022, University of Central Florida, Orlando FL. Paper 1B08.
- AIChE Annual Meeting, Boston MA, November 15-20, 2021.**
- P359. Y. Luo, P. R. Westmoreland, "Aligning What Industry and Academia Expect of New Graduates" in a plenary session "Academia-Industry Partnership: The Undergraduate Curriculum." Paper 96a. **[Invited]**
- P358. C. J. McGill, P. R. Westmoreland, "Mechanism for the Catalysis of Transesterification Using Homogeneous Tin." Paper 616d.
- P357. Y. Tian, G. Luongo, F. Donat, C. R. Müller, P. R. Westmoreland, F. Li, "Oxygen Non-stoichiometry and Defect Models of Brownmillerite-Structured $\text{Ca}_2\text{MnAlO}_{5+\delta}$ for Chemical Looping Air Separation." Paper 736a.
- P356. P. R. Westmoreland, "Opening Lecture: Future Directions of Chemical Engineering as a Transdisciplinary Profession." 18th Brazilian Meeting on Chemical Engineering Education (ENBEQ), 10/24-10/25/2021, Gramado, Brazil. **[Invited]**
- P355. P. R. Westmoreland, "Featured Lecture: Fundamental Reaction Mechanisms of Woody-Biomass Pyrolysis for Engineering Application," 23rd Brazilian Chemical Engineering Congress (COBEQ), 10/26-10/28/2021, Gramado, Brazil. **[Invited]**
- 12th U.S. National Combustion Meeting, Texas A&M University, May 24-26, 2021.**
- P354. A. Jain, A. Bose, P.R. Westmoreland, "Toward Elementary Chemical Mechanisms of Pyrolysis Biofuel Production: Pyrolyzing Hemicellulose Monosaccharides," Paper 1F02.
- P353. Y. Tian, C.J. Montevicchi, F. Li, P.R. Westmoreland, "Probing the Reaction Mechanisms of Chemical Looping - Oxidative Dehydrogenation of Ethane using Molecular-Beam Mass Spectrometry and TGA," Paper 1C12.
- P352. P. R. Westmoreland, "Future Needs for Chemical Engineering Education," NASEM Chemical Engineering Study, Education Subcommittee, 3/11/2021. **[Invited]**
- P351. P. R. Westmoreland, "Applying Molecular Principles toward Reducing Adverse Climate Impacts," 2021 University Research Symposium: Climate Change and Resilience, N. C. State Univ., 3/23/2021.
- P350. P. R. Westmoreland, "Predicting and Measuring Reaction Kinetics of Polymer Degradation and Synthesis," Virtual Symposium on Staudinger's Legacy: The Chain Growth of Polymer Science at NC State, 12/14/2020.
- AIChE Annual Meeting, San Francisco CA (Virtual), November 15-20, 2020.**
- P349. P. R. Westmoreland, "Leading and Managing Industry-Academia Partnerships and Collaborations, Parts I and II," Management Division, Panel 811a (Part I). **[Invited Panelist]**
- P348. P. R. Westmoreland, "Insights into Biphenyl Synthesis from Benzene Pyrolysis Using Rmg and Quantum Chemistry," Catalysis and Reaction Engineering Division, Paper 608b.
- P347. A. Jain, A. Bose, P.R. Westmoreland, "Understanding Glycolaldehyde Formation from Various Monosaccharides," Forest and Plant Bioproducts Division, Paper 507b.
- P346. Y. Tian, R. B. Dudek, L. Brody, L. Neal, P. R. Westmoreland, F. Li, "Kinetic Studies on Chemical Looping – Oxidative Dehydrogenation of Ethane Using Surface-Modified Mixed Oxides," Topical Conference on Next-Gen Manufacturing, Paper 706h.
- P345. Y. Tian, R. B. Dudek, L. Brody, L. Neal, P. R. Westmoreland, F. Li, "Kinetic Chemical Looping – Oxidative Dehydrogenation of Ethane Using Surface Modified Mixed Oxide Particles: Kinetic Studies and Process Demonstration," Particle Technology Forum, Poster 350a.
- P344. P. R. Westmoreland, "Envisioning Changes in Chemical Engineering during the Next 25 Years," 23rd Brazilian Chemical Engineering Congress (COBEQ), Conference Preview Lecture, November 12, 2020. **[Invited]**
- Eastern States Section of the Combustion Institute, Spring Technical Meeting, March 8-11, 2020, Columbia, SC.**
- P343. A. Bose, P.R. Westmoreland, "Dioxane ring formation during xylan torrefaction," Paper 1A03.
- P342. V. Mascarenhas, P. R. Westmoreland, "Estimating flammability limits using predictive modeling of laminar flame speeds," Paper 1B04.

Schoenborn Graduate Research Symposium, Raleigh NC, January 27, 2020.

- P341. Ankush Jain, Arnab Bose, P.R. Westmoreland, "Comparing Pyrolysis of D-Arabinose and L-Fucose to D-Xylose."
- P340. Yuan Tian, P.R. Westmoreland, F. Li, "Reduction kinetics of $\text{CaMn}_{0.9}\text{Fe}_{0.1}\text{O}_3$ for selective hydrogen combustion under a cyclic redox scheme."

AIChE Annual Meeting, Orlando FL, November 10-15, 2019.

- P339. P. R. Westmoreland, "RAPID Manufacturing Institute and AIChE," Paper 7a.
- P338. L.M. Neal, P. R. Westmoreland, H. H. Lamb, T. Fang, F. Li, "Modular Conversion of Stranded Ethane to Liquids," RAPID Poster Session.
- P337. P. R. Westmoreland, "Impacts on Management from an Evolving World and Profession," AIChE Management Award Recipient Presentation Session: Focusing on Technology and Innovation Management, Paper 310b. **[Invited.]**
- P336. P. R. Westmoreland, "A Twenty-Five Year Perspective on Differences and Possibilities in the Practical Adoption of Molecular Simulations Vs Computational Quantum Chemistry," Paper 729a **[Invited]**
- P335. A. Raghu, G. Janarthanam, P. R. Westmoreland, "Reaction Paths Predicted for Xylose and Xylan Pyrolysis Chemistry Using Reactive Molecular Dynamics," Paper 291b.
- P334. A. Jain, A. Bose, P.R. Westmoreland, "Comparing Pyrolysis of D-Arabinose and L-Fucose to D-Xylose," Paper 35d.
- P333. A. Bose, E. Heckard, P.R. Westmoreland, "Degradation kinetics of a liquid mineral oil," Paper 37d.
- P332. P. R. Westmoreland, "Chemical Engineering Developments: Smart Manufacturing." Science Heritage Institute "Innovation Day," Philadelphia PA, September 10, 2019.
- P331. P.R. Westmoreland, A. Bose, C.J. McGill, A. Raghu, "Elementary-Reaction Kinetics for Cellulose and Hemicellulose Pyrolysis," 11th International Conference on Chemical Kinetics, Orléans, France, June 23-27, 2019.

AIChE Annual Meeting, Pittsburgh PA, October 28 - November 2, 2018.

- P330. Clare McCabe, P. R. Westmoreland, "25 by 25: Chemical Engineering in the Next 25 Years." Plenary session "110 years of AIChE". Paper 334a. **[Invited]**
- P329. P. R. Westmoreland, "The future of chemical engineering itself." Plenary session "110 years of AIChE". Paper 334b. **[Invited]**
- P328. A. Raghu, P. R. Westmoreland, "Reaction Paths for Hemicellulose Pyrolysis Using Reactive Molecular Dynamics." Paper 738e.
- P327. C.J. McGill, S. J. Taylor, P. R. Westmoreland, "Homogeneous Catalysis of Ketene Production by Triethylphosphate." Paper 448h.
- P326. C.J. McGill, S. J. Taylor, P. R. Westmoreland, "Mechanism Development for Catalyzed Ketene Production." Poster 189as.
- P325. V.P. Haribal, L. Neal, P. R. Westmoreland, F. Li, "Modeling the Kinetics of Ethane Oxidative Dehydrogenation Via Chemical Looping." Poster 544dz.
- P324. P. R. Westmoreland, "Pericyclic Chemistry in the Anomerization and Pyrolysis of Mono- and Polysaccharides," 6th International Conference on Biomass Energy (ICBE 2018), Wuhan, China, October 16-19, 2018., Paper E1-1. **[Invited lecture.]**
- P323. A. Bose, P. R. Westmoreland, "Understanding the Pyrolysis Kinetics of Xylan and D-Xylose," Thermal & Catalytic Sciences Symposium 2018, Auburn University, Auburn, AL, October 8-10, 2018.
- P322. P.R. Westmoreland, "Using mechanism generators to probe THF combustion chemistry," 4th Workshop on Flame Chemistry, Dublin, Ireland, July 27-28, 2018, Paper 3-4.
- P321. Y. Fenard, A. Gil, G. Vanhove, H.-H. Carstensen, K. M. Van Geem, P. R. Westmoreland, O. Herbinet, F. Battin-Leclerc, "A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants," Workshop: Gas-phase Reaction Kinetics of Biofuels Oxygenated Molecules, Politecnico di Milano, Italy, April 2018.
- P320. A. Bose, P. R. Westmoreland, "Understanding the Pyrolysis Kinetics of Xylan and D-Xylose," 13th Annual Graduate Student Research Symposium, North Carolina State University, Raleigh NC, 2018.

AIChE Annual Meeting, Minneapolis MN, October 29 - November 3, 2017.

- P319. P. R. Westmoreland, "Molecular Modeling of Pyrolysis," Topical Conference on Thermal Deconstruction of Biomass, paper 556a. **[Invited]**

- P318. A. Bose, P. R. Westmoreland, "Analyzing the Torrefaction Products of Galactomannan and Its Monosaccharide Constituents," Poster 639i.
- P317. A. Bose, P. R. Westmoreland, "Measuring the Torrefaction Products of Xylan and D-Xylose" paper 446f.
- P316. C.J. McGill, P. R. Westmoreland, "Pericyclic Reactions in Xylose Pyrolysis and Implications for Xylan Pyrolysis," Poster 639h.
- P315. C.J. McGill, P. R. Westmoreland, "Mechanism Development for the Generation of Furfural in Xylose Pyrolysis," paper 174g.
- 9th Sino-US Joint Conference of Chemical Engineering, Beijing, China, October 15-19, 2017.**
- P314. P.R. Westmoreland. "Molecular Understanding of Woody-Biomass Pyrolysis and Its Yields of Chemicals and Bio-Oils," Paper S11-K3 [Invited keynote speech].
- P313. P.R. Westmoreland. Plenary Panel on the Future Outlook of Chemical Engineering Education.
- P312. P.R. Westmoreland. Plenary Panel of Chemical Engineering Leaders: "Discipline Development Trend of Chemical Engineering in US and China." Paper S13-I11.
- P311. P. R. Westmoreland, "Developing an intellectual and educational framework for modular process intensification," First International Process Intensification Conference, Oct. 1-5, 2017, Barcelona, Spain, Paper 42356.
- P310. P. R. Westmoreland, "Putting chemistry in the chemical engineering curriculum," ASEE Summer School for Chemical Engineering Faculty, July 29 – Aug. 3, 2017, Raleigh, NC.
- P309. C.D. Needham, P.R. Westmoreland, "F-atom chemistry in a hydrogen-starved tetrafluoropropene flame," 10th International Conference on Chemical Kinetics, Chicago, May 21-25, 2017.
- P308. P.R. Westmoreland, M. Day, "Big Data and Analytics for Green Combustion RD&D," NSF Workshop on Combustion Research to Mitigate Carbon Emissions, April 26-27, 2017, College Park Marriott Hotel & Conference Center, Hyattsville MD.
- P307. P.R. Westmoreland, A. Bose, C.J. McGill, "Importance of Pericyclic Reactions for Biomass Pyrolysis and Combustion," U.S. National Combustion Meeting, April 23-26, 2017, College Park Marriott Hotel & Conference Center, Hyattsville MD, Paper 1A07.
- P306. National Academy of Engineering Workshop on Engagement of Engineering Societies in Undergraduate Engineering Education, Keck Center, Washington DC, January 25-26, 2017.
P.R. Westmoreland, "Academic-Industry Alignment on Expectations of New ChE Graduates."
P.R. Westmoreland, "AIChE's aid to new emphases on ChE process safety."
P.R. Westmoreland, "AIChE's engagement through the Manufacturing USA institutes CESMII and RAPID,"
- P305. P.R. Westmoreland, "Developing an intellectual and educational framework for modular process intensification" NSF/DOE Modular Manufacturing Workshop, Holiday Inn Arlington, Arlington VA, January 17-18. 2017.
- AIChE Annual Meeting, San Francisco CA, November 13-18, 2016.**
- P304. V. Seshadri, P. R. Westmoreland, "Pyrolysis Kinetics to and from Levoglucosan," Paper 432d.
- P303. S. J. Taylor, P. R. Westmoreland, H. Key, "Gas-Phase Catalysis for Pyrolyzing Acetic Acid," Paper 375c.
- Symposium on Thermal and Catalytic Sciences for Biofuels and Biobased Products, Chapel Hill NC, November 1-3, 2016.**
- P302. P. R. Westmoreland, P.J. Fahey, V. Seshadri, "Pyrolysis of Two- and Three-Carbon Monosaccharides to Understand Hemicellulose and Cellulose Pyrolysis."
- P301. C. J. McGill, P. R. Westmoreland, "Establishing Elementary Reactions of Hemicellulose Torrefaction."
- P300. P.R. Westmoreland, S. Baskaran, M.P. Burke, M. Frenklach, C.D. Needham, J. Oreluk, U. Riedel, S.M. Sarathy, N. Slavinskaya, R.H. West, "Developing Combustion Mechanisms Dynamically as a Community," 36th International Symposium on Combustion, Seoul, Republic of Korea, July 31-August 5, 2016, Poster 04P017.
- P299. P.R. Westmoreland, "Cyberinfrastructure and big data," 3rd International Workshop on Flame Chemistry, Prima Hotel, Seoul, Republic of Korea, July 30-31, 2016. **[Invited]**
- P298. P.R. Westmoreland, P.J. Fahey, "Dehydration and dehydrogenation kinetics of OH groups in biomass pyrolysis," 2nd International Conference on Biomass, Giardini Naxos-Taormina, Sicily, Italy, June 19-22, 2016.

- P297. P.R. Westmoreland, "R-OH hydroxyl catalysis of pyrolysis reactions," 21st International Symposium on Analytical and Applied Pyrolysis, Nancy, France, May 9-12, 2016.
AIChE Annual Meeting, Salt Lake City UT, November 8-13, 2015.
- P296. P. R. Westmoreland, "Preparing Graduate Students for Their Careers," Paper 113b.
- P295. P. R. Westmoreland, S. D. Crymble, S. J. Taylor, and C. J. McGill, "Pyrolysis of fuels to absorb heat before use in combustion," Paper 315a.
- P294. P. J. Fahey, P. R. Westmoreland, "Thermal Conversion Pathways for Simple Sugars." Paper 684c.
- P293. P. R. Westmoreland, S. D. Crymble, S. J. Taylor, C. J. McGill. "Pyrolysis of fuels to absorb heat before use in combustion," Division of Energy and Fuels, 250th National Meeting of the American Chemical Society, Boston MA, August 16-20, 2015, Paper ENFL-353.
- P292. C.D. Needham, E. C. Dandley, G. N. Parsons, P. R. Westmoreland, "Molecular Modeling of Reactive Systems for the Exploration and Development of Reaction Mechanisms," Foundations of Molecular Modeling and Simulation, The Resort at Mt. Hood, OR, July 12-16, 2015.
- P291. C.D. Needham, N.J. Labbe, T.G. Voskuilen, T.L. Pourpoint, P.R. Westmoreland, "An Extended Mechanism for the Hypergolic Combustion of Monomethylhydrazine and Nitric Acid," U.S. National Combustion Meeting, May 17-20, 2015, Cincinnati, OH, paper 2G03.
- P290. P. R. Westmoreland, "Measuring Kinetics of Hydrocarbon and Oxygenate Pyrolysis," Murphree Award Symposium in Honor of Joseph R. Zoeller, 249th National Meeting of the American Chemical Society, Denver CO, March 24, 2015. **[Invited lecture.]**
- P289. C.D. Needham, P. R. Westmoreland, "The Role of Aerosols in Hypergolic Ignition," AIChE Annual Meeting, Atlanta GA, November 16-21, 2014, paper 528c.
- P288. P. R. Westmoreland, "Process Intensification: Concepts and Applications," NSF Workshop on Process Intensification, Arlington VA, Sept. 29-Oct. 1, 2014. **[Invited lecture.]**
- P287. P. R. Westmoreland, "Making Bio-oils: A Microcosm of the Opportunities and Challenges for a Golden Age of ChE," 21st International Congress of Chemical and Process Engineering (CHISA 2014) and 17th Conference on Process Integration, Modeling, and Optimisation for Energy Saving and Pollution Reduction (PRES 2014), Prague, Czech Republic, August 23-27, 2014. **[Invited Keynote Address.]**
- P286. V. Seshadri, P. J. Fahey, P.R. Westmoreland. "Role of pericyclic reactions in the pyrolysis of cellulose and hemicellulose," 248th National Meeting of the American Chemical Society, San Francisco CA, August 10-14, 2014. **[Invited keynote.]**
- P285. P.R. Westmoreland, "Elementary-Reaction Kinetics for Engineering the Pyrolysis and Combustion of Gas, Biomass, Synthetic Polymers, & Coal," Joint NSF-NSFC Workshop on Combustion Related to Sustainable Energy, Hangzhou, China, March 10-12, 2014. **[Invited]**
- P284. P.R. Westmoreland. "Opportunities and Challenges in a New Golden Age of Chemical Engineering," Bob Bird 90th Birthday Symposium, University of Wisconsin - Madison, January 30-31, 2014. **[Invited]**
AIChE Annual Meeting, San Francisco CA, November 3-8, 2013:
- P283. V. Seshadri, P. J. Fahey, X. Geng, P. R. Westmoreland, "Pyrolysis Kinetics for Small-Molecule Intermediates of Cellulose Pyrolysis," paper 27a.
- P282. P. J. Fahey, V. Seshadri, X. Geng, P. R. Westmoreland, "Reactant Conversion and Product Speciation of Carbohydrate Model-Compound Pyrolysis Using a Novel Flow Reactor," paper 147b.
- P281. P.R. Westmoreland. "Entering a Golden Age of Chemical Engineering," AIChE National Capital Local Section Meeting, October 30, 2013. **[Invited]**
- P280. P.R. Westmoreland. "Frontiers of Chemical Engineering," 7th Sino-US Joint Conference of Chemical Engineering, Beijing, China, October 14-18, 2013. **[Invited plenary speech/discussion participant.]**
Eastern States Section of the Combustion Institute, October 13-16, 2013, Clemson, SC.
- P279. C.D. Needham, P.R. Westmoreland, "Using Reactive Molecular Dynamics Simulations to Refine the Mechanism of TMEDA Combustion," paper B12.
- P278. P.J. Fahey, V. Seshadri, P.R. Westmoreland. "Dehydrogenation Activity in Low-Temperature Gas-Phase Alcohol Pyrolysis," paper B19.
- P277. V. Seshadri, W. Li, P.R. Westmoreland. "Species measurements in a low-pressure, fuel-rich JP-10/H₂ flat flame," paper A21.

- P276. P.R. Westmoreland. "Fundamental Kinetics for Pyrolysis of Lignocellulosic Biomass to Bio-oil," 2nd Middle East Process Engineering Conference, 9/29-10/2/2013. **[Invited.]**
- P275. P.R. Westmoreland. "Opportunities and Challenges in a New Golden Age of Chemical Engineering," 2nd Middle East Process Engineering Conference, 9/29-10/2/2013. **[Invited Keynote Address.]**
- P274. P.R. Westmoreland. "Molecular Kinetics of Making Bio-oils: Opportunities and Challenges for a Golden Age of ChE," Jahrestreffen der Fachgemeinschaft Fluidodynamik und Trenntechnik 2013, Würzburg, Germany, September 24-27, 2013. **[Invited plenary address.]**
- P273. P.R. Westmoreland. "Entering a Golden Age of Chemical Engineering," AIChE Eastern North Carolina Local Section Meeting, September 18, 2013. [Invited]
- P272. P.R. Westmoreland. "Fundamental Kinetics for Pyrolysis of Lignocellulosic Biomass to Bio-oil," World Congress of Chemical Engineering, incorporating 15th Asian Pacific Confederation of Chemical Engineering Congress, Seoul, Korea, August 19-23, 2013. **[Invited.]**
- P271. P.R. Westmoreland. "Entering a Golden Age of Chemical Engineering," AIChE Baton Rouge Local Section Meeting, April 8, 2013. **[Invited]**
- P270. P.R. Westmoreland, "Elementary-reaction kinetics for making and burning biomass-derived fuels," Abstracts of Papers of the American Chemical Society, vol. 245, published April 7, 2013; **Invited talk** at 245th National Spring Meeting of the American Chemical Society.
- P269. P.R. Westmoreland. "Entering a Golden Age of Chemical Engineering," AIChE Virtual Local Section Meeting, January 24, 2013. **[Invited]**
- AIChE Annual Meeting, Pittsburgh PA, October 28-November 2, 2012:**
- P268. N. Labbe, P.R. Westmoreland. "Modeling ammonia combustion to develop a comprehensive reaction set for N/H/O kinetics."
- P267. P.J. Fahey, V. Seshadri, P. R. Westmoreland, "Insights from glucose pyrolysis for cellulose pyrolysis."
- P266. P.R. Westmoreland. "Opening remarks: Symposium in honor of Keith Gubbins' 75th birthday."
- P265. P.R. Westmoreland, "Plans for a National Combustion-Data Cyberinfrastructure," MACCCR Fuels Summit, Sandia National Laboratories, September 17, 2012 [Invited].
- 34th International Combustion Symposium, Warsaw University of Technology, Warsaw, Poland, July 29-August 3, 2012.**
- P264. N. J. Labbe, V. Seshadri, T. Kasper, N. Hansen, P. Oßwald, P. R. Westmoreland, "Flame chemistry of tetrahydropyran as a model heteroatomic biofuel," Podium presentation.
- P263. T. Bierkandt, T. Kasper, N. Labbe, P.R. Westmoreland, D.A. Knyazkov, S.A. Yakimov, O.P. Korobeinichev, "Effect of nitrogen addition to low-pressure, premixed flat ethanol flames," poster.
- P262. **Foundations of Molecular Modeling and Simulation, The Resort at Mt. Hood, OR, July 22-26, 2012.**
- P. R. Westmoreland. "Modeling Biofuel Products and Processes." **[Invited.]**
- P261. N. Labbe and P.R. Westmoreland. "Flame chemistry of tetrahydropyran as a model heteroatomic biofuel," 30th Regional Meeting on Chemical Kinetics and Dynamics, SUNY-Albany, Albany NY, January 28, 2012.
- AIChE Annual Meeting, Minneapolis MN, October 7-12, 2011:**
- P260. N. Labbe, Y. S. Kim, P.R. Westmoreland. "Computational Mechanism Development for Hypergolic Propellant Systems: MMH and DMAZ." Paper (poster and podium).
- P259. K. D. Smith, M. Bruns, S. I. Stoliarov, Marc R. Nyden, O. A. Ezekoye, P. R. Westmoreland, "Analysis of Chain Scission in Polymers Using Reactive Molecular Dynamics."
- P258. V. Seshadri, J. R. Keith, P.R. Westmoreland. "Predictions of elementary reactions for pyrolysis of glucose." Paper 712f.

Fall Technical Meeting, Eastern Section of the Combustion Institute, Univ. of Connecticut, Storrs CT, October 9-12, 2011:

- P257. W. Li, P. R. Westmoreland, B. Yang, N. Hansen. "Molecular-weight growth in fuel-rich toluene + methane and toluene + acetylene flames." Paper B-10.
- P256. W. Li, P. R. Westmoreland, B. Yang, N. Hansen. "Stoichiometric effects on oxidation and benzene-formation chemistry in premixed 1-hexene flames." Paper A-15.
- P255. X. Yang, C. Chen, P. R. Westmoreland. "Experimental and theoretical study of the reactions of CHF radicals with C₂H₂, C₂H₄, and NO in the temperature range of 296-670 K." Paper A-16.
- P254. N. Labbe, P.R. Westmoreland. "Reaction kinetics for TMEDA combustion with red fuming nitric acid." Paper A-20.
- P253. V. Seshadri, J. R. Keith, P.R. Westmoreland. "Elementary-reaction kinetics of glucose pyrolysis." Paper A-34.

International Conference on Chemical Kinetics, Cambridge MA, March 20-23, 2011.

- P252. P.R. Westmoreland, T. Russi, A. Packard, M. Frenklach, "Uncertainty-quantified analysis of complex experimental data."

7th U.S. National Combustion Meeting, Atlanta GA, March 20-23, 2011.

- P251. D.R. Yeates, W. Li, P.R. Westmoreland, T. Russi, A. Packard, M. Frenklach, "Uncertainty-quantified analysis of complex experimental data."
- P250. W. Li, M.E. Law, P.R. Westmoreland, T. Kasper, N. Hansen, K. Kohse-Höinghaus, "Multiple benzene-formation paths in a fuel-rich cyclohexane flame."
- P249. N. Labbe, A. Lucassen, P.R. Westmoreland, K. Kohse-Höinghaus, "Mechanistic insights into nitrogen fate in a morpholine flat flame."
- P248. A. Lucassen, P. Oßwald, N. Labbe, P. R. Westmoreland, K. Kohse-Höinghaus, "Combustion Behavior of Nitrogen-Containing Model Biofuels," Annual Convention of the Deutschen Gesellschaft für Massenspektrometrie, February 27-March 2, 2011.
- P247. N. Labbe and P.R. Westmoreland. "New developments in morpholine flame modeling and mechanism development," 29th Regional Meeting on Chemical Kinetics and Dynamics, University of Massachusetts Amherst, January 29, 2011.

AIChE Annual Meeting, Salt Lake City UT, November 7-12, 2010:

- P246. N. Labbe, Y. S. Kim, P.R. Westmoreland. "Computational Mechanism Development for Hypergolic Propellant Systems: MMH and DMAZ." Paper (poster and podium).
- P245. K. D. Smith, M. Bruns, S. I. Stoliarov, Marc R. Nyden, O. A. Ezekoye, P. R. Westmoreland, "Analysis of Chain Scission in Polymers Using Reactive Molecular Dynamics."
- P244. W. Li, B. Yang, P. R. Westmoreland, B. Yang, T. Kasper, N. Hansen. "Comparison of Fuel-Rich and Stoichiometric Premixed Toluene Flames." Paper.
- P243. "Innovation and Insight via High-Fidelity Simulation and Large-Database Studies of Micro, Macro and Multi-Scale Phenomena": Introduction and Session Objectives (with Sharon Glotzer and Peter Cummings) and Open Discussion on High-Performance Computing in Chemical Engineering (with Sharon Glotzer and Peter Cummings).
- P242. C. Cooper and P.R. Westmoreland, "Federal Agency View of Simulation-Based Engineering and Science."
- P241. W. Li, M. E. Law, P. R. Westmoreland, M. E. Law, T. Kasper, N. Hansen, J. Wang, T. A. Cool, K. Kohse-Höinghaus. "Competing paths for benzene formation in cyclohexane premixed flat flames," 33rd International Symposium on Combustion, Beijing, China, Aug. 1-6, 2010. Work-in-Progress poster WP5006.
- P240. A. Lucassen, P. Oßwald, U. Struckmeier, K. Kohse-Höinghaus, T. Kasper, N. Hansen, N. Labbe, P. R. Westmoreland, T. A. Cool, "Fuel-Nitrogen Conversion of Model Biofuels," Annual Meeting of the Bunsen Society, May 2010 (poster and abstract).
- P239. N. Labbe and P.R. Westmoreland. "New developments in morpholine flame modeling and mechanism development," 28th Regional Meeting on Chemical Kinetics and Dynamics, Trinity College, Hartford CT, January 30, 2010.

AIChE Annual Meeting, Nashville TN, November 8-13, 2009:

- P238. N. Labbe, P.R. Westmoreland, A. Lucassen, P. Oßwald, U. Struckmeier, K. Kohse-Höinghaus, T. Kasper, N. Hansen, T.A. Cool. "Mechanism Development for Combustion of Morpholine." Papers 178k (poster) and 399d (podium).

- P237. W. Li, N. Labbe, P. R. Westmoreland, B. Yang, J. Wang, T. A. Cool, T. Kasper, N. Hansen, K. Kohse-Höinghaus, Bielefeld University. "Inferring Fuel-Rich Toluene Flame Chemistry From Photo-Ionization MBMS Analysis and Modeling." Paper 673e.
- P236. N. Labbe, P.R. Westmoreland. "Understanding Polymer Pyrolysis through Advances in Reactive Molecular Simulation," Fall Technical Meeting, Eastern Section of the Combustion Institute, Univ. of Maryland, College Park, October 18-21, 2009.
- P235. P.R. Westmoreland. "Chemical Engineering Challenges and Opportunities in Simulation-Based Science and Engineering," 5th Sino-U.S. Conference of Chemical Engineering, Beijing, China, October 12-16, 2009. **Invited.**
- P234. **Foundations of Molecular Modeling and Simulation, Blaine WA, July 12-16, 2009.**
P. R. Westmoreland, N. Labbe. "Applying Computational Quantum Chemistry to Devise a Combustion Mechanism for Morpholine, a Biofuel Surrogate."
- P233. **20th Annual BCC Conference on Flame Retardancy, Stamford CT, June 1-3, 2009.**
R. Mosurkal, J. W. Soares, R. Kirby, W. Muller, L. A. Samuelson, P. R. Westmoreland, J. Kumar. "Novel Organic-Inorganic Hybrid Copolymers as Environmentally Safe Flame-Retardant Materials."
6th U.S. National Combustion Meeting, Ann Arbor, May 17-21, 2009.
- P232. B. Yang, J. Wang, T.A. Cool, T. Kasper, N. Hansen, K. Kohse-Höinghaus, P.R. Westmoreland. "MBMS Study of Low-Pressure Premixed C₅H₁₀O₂ Ethyl and Methyl Ester Flames."
- P231. N. Hansen, J. A. Miller, P. R. Westmoreland, T. Kasper, K. Kohse-Höinghaus, J. Wang, T. A. Cool. "Isomer-Specific Combustion Chemistry in Allene and Propyne Flames."
- P230. W. Li, M.E. Law, P.R. Westmoreland, T. Kasper, N. Hansen, T.A. Cool, K. Kohse-Höinghaus. "Photo-ionization MBMS Analysis and Modeling of a Fuel-Rich Cyclohexane Flame."
- P229. P.R. Westmoreland, W. Li, N. Hansen, T. Kasper, T.A. Cool, A. Lucassen, K. Kohse-Höinghaus. "Advances in understanding ethyne chemistry from 45 years of MBMS flame research."
- P228. P.R. Westmoreland, "High-Impact Research Invited Talk: Overview of NSF's View of Cutting-Edge Chemical Engineering Research." AIChE Spring National Meeting, Tampa FL, April 26-30, 2009. **Invited.**
- P227. P.R. Westmoreland, "Developing the promise of Reactive Molecular Dynamics for performing kinetics experiments computationally." 237th ACS National Meeting, Salt Lake City UT, March 22-26, 2009. **Invited.**
27th Regional Meeting on Chemical Kinetics and Dynamics, Univ. of Massachusetts Amherst, January 31, 2009:
- P226. N. Labbe and P.R. Westmoreland. "Morpholine flame modeling and mechanism development."
- P225. W. Li and P.R. Westmoreland. "Measurement and modeling of fuel-rich cyclohexene combustion."
- AIChE Annual Meeting, Philadelphia PA, November 16-21, 2008:**
- P224. P.R. Westmoreland, S.V. Tulyani, K.D. Smith, M.R. Nyden, S.I. Stoliarov, G. A. Petersson. "Advances toward Obtaining Kinetics from Reactive Molecular Dynamics." Paper 96e. **Invited.**
- P223. P.R. Westmoreland. "An International Assessment of R&D In Simulation-Based Engineering and Science: Introduction: Introduction and Discussion." Paper 709c and 709d.
- P222. P.R. Westmoreland. "Using Cyberinfrastructure to Weave Combustion Data and Models into Engineering Solutions." International Mechanical Engineering Conference, Boston MA, November 3-7, 2008. Paper IMEC2008-69299. **Invited.**
- P221. S. Tulyani, P. R. Westmoreland, G. A. Petersson. "BEBOP, A New Reactive Potential using Bond-Energy/Bond-Order Relationships." World Association of Theoretical and Computational Chemists, Sydney Convention and Exhibition Centre, Sydney, Australia, September 14-19, 2008. Poster PP012.
- P220. N. Labbe, W. Li, P.R. Westmoreland, A. Lucassen, P. Oßwald, U. Struckmeier, K. Kohse-Höinghaus, T. Kasper, N. Hansen, T.A. Cool. "Development of a combustion mechanism for morpholine. " 32nd International Symposium on Combustion, Montreal, Canada, August 3-8, 2008. Poster W5P111.
- P219. P. R. Westmoreland, M. Chaos, T. A. Cool, F. L. Dryer, N. Hansen, T. Kasper, K. Kohse-Höinghaus, M. E. Law, W. Li, P. Oßwald, U. Struckmeier, C. K. Westbrook, B. Yang, J. Wang, "Using MBMS for Characterization and Kinetics in Hydrocarbon and Oxygenate Flames", Central States Spring Technical Meeting, University of Alabama, April 20-22, 2008. Paper A-2a.

- 26th Regional Meeting on Chemical Kinetics and Dynamics, SUNY, Albany NY, January 26, 2008:**
- P218. K. Smith and P.R. Westmoreland. "Understanding the effects of polymer architecture on the backbone scission kinetics."
- P217. S. Tulyani and P.R. Westmoreland, "BEBOP, A New Reactive Potential using Bond-Energy/Bond-Order Relationships."
- P216. N. Labbe and P.R. Westmoreland, "Determining the Kinetics of C₃H₂ and C₃H₃ Reactions Using Ab Initio Methods."
- AIChE Annual Meeting, Salt Lake City UT, November 1-9, 2007:**
- P215. K.D. Smith, S.I. Stoliarov, M.R. Nyden, P.R. Westmoreland. "Understanding Polymer Pyrolysis through Advances in Reactive Molecular Simulation." Paper 77b.
- P214. S. Tulyani, P.R. Westmoreland, G.A. Petersson, "BEBOP, A New Reactive Potential Using Bond-Energy/Bond-Order Relationships." Paper 469a.
- P213. Lam K. Huynh, Hongzhi R. Zhang, Eric G. Eddings, Adel F. Sarofim, Phillip R. Westmoreland, Thanh N. Truong, "Kinetics of Enol Formation from Reaction of OH with Propene." Paper 580c.
- 2007 Fall Meeting of the Western States Section of the Combustion Institute, Livermore CA, October 16-17, 2007:**
- P212. P.R. Westmoreland. "Recent Advances in Flame-Sampling Molecular-Beam Mass Spectrometry." **[Invited plenary lecture.]**
- P211. T. Kasper, N. Hansen, J. Wang, B. Yang, T.A. Cool, P.R. Westmoreland. "MBMS investigation of a laminar tetrahydrofuran flame." Paper 07F-8.
- P210. N. Hansen, S. J. Klippenstein, P. R. Westmoreland, T. Kasper, K. Kohse-Höinghaus, J. Wang, and T. Cool. "Combined ab initio and Photoionization Mass Spectrometric Study of Polyynes in Fuel-Rich Flames." Paper 07F-31.
- P209. S. Tulyani, P.R. Westmoreland, M.J. Frisch, E.J. Petersson, G.A. Petersson, "BEBOP, A New Reactive Potential Using Bond-Energy/Bond-Order Relationships," 234th ACS National Meeting, Boston, MA, August 19-23, 2007. Paper COMP 075, Division of Computers in Chemistry.
- P208. S.I. Stoliarov, K.D. Smith, P.R. Westmoreland, R.E. Lyon, M.R. Nyden, "A new reactive molecular dynamics model of polymer pyrolysis," Proceedings of the 18th Annual BCC Research Conference on Recent Advances in Flame Retardancy of Polymeric Materials, Stamford CT, May 21-23/2007, pp 1-8.
- P207. P. R. Westmoreland, "The prehistory of soot: Small rings from small molecules" at Workshop on Combustion Generated Fine Carbonaceous Particles, Villa Orlandi, Anacapri, May 13 - 16, 2007. **Invited keynote.**
- P206. N. Hansen, T. Kasper, S.J. Klippenstein, P.R. Westmoreland, M.E. Law, C.A. Taatjes, K. Kohse-Höinghaus, J. Wang, T.A. Cool. "Fuel Consumption and Initial Steps of Aromatic Ring Formation in a Laminar Premixed Fuel-Rich Cyclopentene Flame," 5th Joint Meeting of the U.S. Sections of the Combustion Institute, San Diego CA, March 25-28, 2007. Paper A09.
- P205. U. Struckmeier, L.-C. Salameh, P. Oßwald, K. Kohse-Höinghaus, J. Wang, T. Cool, N. Hansen, M. Law, P. Teella, P. Westmoreland. "Combustion chemistry of n-butane and iso-butane analyzed by VUV-photoionization mass spectrometry." 40th Diskussionstagung der Deutschen Gesellschaft für Massenspektrometrie, Universität Bremen, Germany, March 11-14, 2007.
- 25th Regional Meeting on Chemical Kinetics and Dynamics, Wadsworth Center, Albany NY, January 27, 2007.**
- P204. K. Smith and P.R. Westmoreland. "Simulating ethane decomposition using Reactive Molecular Dynamics."
- P203. S. Tulyani and P.R. Westmoreland, "Development of a Bond Order Potential (BOP) for Reactive Molecular Dynamics."
- P202. P.R. Westmoreland. "Advances in Fire-Safe Polymers with Novel Experiments and Cyberinfrastructure." Sukant Tripathy Annual Memorial Symposium, Wannalancit Mills Conference Center, Lowell MA, Dec. 1, 2006. **[Invited.]**
- P201. P.R. Westmoreland. "James M. Douglas, Winner of the 2006 ASEE / CACHE Award for Excellence in Computing in Chemical Engineering Education." AIChE Annual Meeting, San Francisco CA, Nov 12-17, 2006. Paper 206a.

- Science Fair im Rahmen der Berufseinstiegsmesse Perspektive_06, Universität Bielefeld, November 3, 2006.**
- P200. U. Struckmeier, T. Kasper, P. Oßwald, K. Kohse-Höinghaus, N. Hansen, C.A. Taatjes, J. Wang, T.A. Cool, S. Gon, P.R. Westmoreland, "Mass-spectrometric investigation of ethanol-blended propene flames."
- P199. P. Oßwald, T. Kasper, K. Kohse-Höinghaus, J. Wang, T. Cool, N. Hansen, C. Taatjes, S. Gon, P. R. Westmoreland, F. Qi, "Isomer-selective molecular-beam mass spectrometric investigation of flames burning oxygenated fuels."
- 232nd National Meeting of the American Chemical Society, San Francisco CA, September 10-14, 2006.**
- P198. R. Mosurkal, V. Tucci, L.A. Samuelson, F. Bruno, P.R. Westmoreland, V.S. Parmar, J. Kumar, A.C. Watterson. "Biocatalytic synthesis of organic-siloxane copolymers for flame-retardant applications." Paper POLY 533.
- P197. M. Frenklach, A. Packard, Z. M. Djuricic, R. Feeley, T. Russi, D. M. Golden, A. Gupta, C. T. Bowman, W. H. Green, G. J. McRae, P. J. Smith, H. Wang, P. R. Westmoreland, T. C. Allison, J. Frey, M. J. Pilling, "Process informatics for chemical reaction systems." Paper PHYS 277.
- 31st International Symposium on Combustion, Heidelberg, Germany, August 6-11, 2006.**
- P196. N. Hansen, P.R. Westmoreland, L. Rahn. "A Web-based library of low-pressure flame data." Work-in-progress poster 4C-26, page 419.
- P195. T. Kasper, P. Oßwald, K. Kohse-Höinghaus, C.A. Taatjes, J. Wang, T. A. Cool, M.E. Law, A. Morel, P.R. Westmoreland. "Isomeric propanol flames investigated by mass spectrometry." Work-in-progress poster 4C-22, page 415.
- P194. P. Oßwald, U. Struckmeier, T. Kasper, K. Kohse-Höinghaus, N. Hansen, C.A. Taatjes, J. Wang, T. A. Cool, S. Gon, P.R. Westmoreland. "Experimental study of premixed propene/ethanol blends." Work-in-progress poster 4C-09, page 402.
- P193. P. Oßwald, T. Kasper, K. Kohse-Höinghaus, J. Wang, T. A. Cool, N. Hansen, P.R. Westmoreland. "Studies of the chemistry of fuel-rich methyl acetate and ethyl formate flames with photoionization mass spectrometry." Work-in-progress poster 2D-11, page 281.
- P192. K.D. Smith, S.I. Stoliarov, M.R. Nyden, P.R. Westmoreland. "RMDff: A Smoothly Transitioning, Forcefield-Based Representation of Kinetics for Reactive Molecular Dynamics Simulations." Foundations of Molecular Modeling and Simulation, Semiahmoo Resort, Blaine WA, July 9-14, 2006.
- P191. H.R. Zhang, L.K. Huynh, N. Kungwan, S. Zhang, Z. Yang, T.N. Truong, E.G. Eddings, A.F. Sarofim, M. Law, P.R. Westmoreland. "Enol Formation in a Stoichiometric Cyclohexane Flame." 231st National Meeting of the American Chemical Society, Atlanta GA, March 26-30, 2006.
- P190. P.R. Westmoreland. "New Approaches for Teaching the Chemical Principles of Engineering." Paper 2D-1. American Society for Engineering Education New England Section Annual Conference, Worcester (MA) Polytechnic Institute, March 18, 2006. **Invited.**
- 105th Hauptversammlung der Deutschen Bunsen-Gesellschaft für Physikalische Chemie (Bunsentagung), Friedrich-Alexander-Universität, Erlangen Germany, January 29 - February 3, 2006.**
- P189. P. Oßwald, T. Kasper, K. Kohse-Höinghaus, J. Wang, T. Cool, N. Hansen, C. Taatjes, S. Gon, P. R. Westmoreland, F. Qi, "Combustion of oxygenated fuels – comparison of isomeric fuels."
- P188. P. Oßwald, T. Kasper, K. Kohse-Höinghaus, J. Wang, T. Cool, N. Hansen, C. Taatjes, S. Gon, P. R. Westmoreland, F. Qi, "Isomer-selective molecular-beam mass spectrometric investigation of flames burning oxygenated fuels."
- P187. U. Struckmeier, T. Kasper, P. Oßwald, K. Kohse-Höinghaus, N. Hansen, C. Taatjes, J. Wang, T. Cool, S. Gon, P. R. Westmoreland, "Combustion chemistry of ethanol-blended propene flames."
- P186. N. Hansen, S.J. Klippenstein, C. A. Taatjes, T. A. Cool, J. Wang, T. Kasper, K. Kohse-Höinghaus, M. E. Law, P. R. Westmoreland, F. Qi, "Synchrotron Photoionization Molecular-Beam Mass Spectrometric Characterization of Hydrocarbon Radicals in Fuel-Rich Flames." 4th Gordon Research Conference on Photoions, Photoionization and Photodetachment, Buellton CA, January 29 - February 3, 2006.
- 24th Regional Meeting on Chemical Kinetics and Dynamics, Rensselaer Polytechnic Institute, Troy NY, January 28, 2006.**
- P185. S. Tulyani and P.R. Westmoreland, "Development of an EHT-BEBO Method for Calculation of Potential Surfaces near the Transition State."

- P184. K. Smith and P.R. Westmoreland. "Development of Smoothly Transitioning Forcefield-Based Method for Reactive Molecular Dynamics."
- P183. S. Gon and P.R. Westmoreland. "MBMS Study of a Fuel-rich Cyclohexane Flame."
- P182. M.R. Nyden, S.I. Stoliarov, P.R. Westmoreland, and V.D. Knyazev, "Simulating Chemical Reactions Involving Large Molecules and Nanostructures." International Conference on Computational & Experimental Engineering and Sciences, Chennai India, Dec. 1-5, 2005. **Invited.**
Fall Technical Meeting, Eastern Section of the Combustion Institute, Univ. of Central Florida, Orlando FL, November 14-16, 2005:
- P181. P.R. Westmoreland. "Recent Advances in Molecular-Beam Mass Spectrometry of Flames." *Chemical and Physical Processes of Combustion*. **Invited Plenary Lecture.**
- P180. M.E. Law, P.R. Westmoreland, T.A. Cool, J. Wang, N. Hansen, C.A. Taatjes, and T. Kasper. "Insights Into a Premixed Stoichiometric Cyclohexane Flame." *Chemical and Physical Processes of Combustion*, 221-224.
- P179. M.E. Law, S. Gon, P.R. Westmoreland, T.A. Cool, J. Wang, N. Hansen, and C.A. Taatjes. "1,5-Hexadiyne and Fulvene Presence in Premixed Allene and Propyne Flames." *Chemical and Physical Processes of Combustion*.
- P178. S. Gon, M.E. Law, P.R. Westmoreland, T.A. Cool, J. Wang, N. Hansen, C.A. Taatjes, T. Kasper, K. Kohse-Höinghaus. "Identification of Species and Separation of Isomers in a Premixed Fuel-Rich Cyclohexane Flame." *Chemical and Physical Processes of Combustion*.
- P177. P.R. Westmoreland. "Applying Molecular Modeling to Identify Pollutant Precursors: C₃H₂'s." Annual Meeting of AIChE, Cincinnati OH, Oct. 30-Nov. 4, 2005. Paper 568c (Invited substitute).
- P176. P.R. Westmoreland, M.E. Law, T.A. Cool, J. Wang, A. McIlroy, C.A. Taatjes, N. Hansen. "Analysis of Flame Structure by Molecular-Beam Mass Spectrometry Using Electron-Impact and Synchrotron-Photon Ionization," Fifth International Seminar on Flame Structure, Novosibirsk Russia, July 11-14, 2005. **Invited Keynote Lecture.**
4th Joint Meeting of the U.S. Sections of the Combustion Institute, Philadelphia PA, March 20-23, 2005:
- P175. M.E. Law, P.R. Westmoreland, T.A. Cool, J. Wang, N. Hansen, C.A. Taatjes, T. Kasper. "Benzene Formation in a Stoichiometric Cyclohexane Flame," Paper B26.
- P174. A. Schoemann, P.R. Westmoreland, H. Q. Zhang, R. J. Farris, R.E. Lyon, R.N. Walters. "A Pyrolysis-Based Method for Characterizing Flammability and Thermal Decomposition of Polymers," Paper E09.
- P173. M.E. Law, P.R. Westmoreland. "New flame measurements from the ALS." 23rd Regional Meeting on Kinetics and Dynamics, University of Massachusetts Amherst, January 28, 2005.
Annual Meeting of AIChE, Austin TX, November 7-12, 2004:
- P172. P.R. Westmoreland. "Homogeneous Reaction and Reactive Flow Modeling." Plenary session of Topical Conference on "Coupling Theory, Molecular Simulations and Computational Chemistry to the Physical World." Paper 43a. **Invited Plenary Lecture.**
- P171. M.R. Nyden. S.I. Stoliarov, P.R. Westmoreland. "Toward the Development of a Method for Predicting the Rates of the Thermal Decomposition of Large Molecules and Nanostructures." Paper 166c. Invited.
- P170. P.R. Westmoreland, M.E. Law, A. Morel, T.A. Cool, C.A. Taatjes. "Toward the Development of a Method for Predicting the Rates of the Thermal Decomposition of Large Molecules and Nanostructures." Paper 550d.
228th ACS National, Meeting of ACS, Philadelphia PA, August 22-26, 2004:
- P169. P.R. Westmoreland. "Obtaining rate constants and mechanisms from flame MBMS." Division of Physical Chemistry, paper 693. **Invited.**
- P168. S.I. Stoliarov, H. Zhang, P.R. Westmoreland, R. E. Lyon, M.R. Nyden. "Molecular modeling of the thermal decomposition of polymers." Division of Polymeric Materials: Science and Engineering, paper 165; *Polymeric Materials Science and Engineering* **91**, 284-85 (2004).
30th International Symposium on Combustion, Univ. of Illinois Chicago, July 26-30, 2004:
- P167. B. Ruscic, J.E. Boggs, A.G. Burcat, A.G. Császár, J. Demaison, R. Janoschek, J.M.L. Martin, M.L. Morton, M.J. Rossi, J.F. Stanton, P.G. Szalay, P.R. Westmoreland, F. Zabel, T. Bérces.

- “IUPAC critical evaluation of thermochemical properties of selected radicals,” WIP poster 1F1-30.
- P166. T. Kasper, M. Letzgus, K. Kohse-Höinghaus, C. A. Taatjes, A. Mcllroy, T. A. Cool, J. Wang, M. E. Law, A. Morel, P. R. Westmoreland, “Investigation of Alcohol Flames by Mass Spectrometry,” poster 4F4-20.
- P165. P. R. Westmoreland, A. Z. Panagiotopoulos. "Molecular-Modeling Methods and Use for Product and Process Design." Foundations of Computer-Aided Process Design, Princeton NJ, July 11-16, 2004. **Invited lecture.**
- P164. S. J. Klippenstein, Y. Georgievskii, J. A. Miller, L. B. Harding, J. A. Nummela, B. K. Carpenter, P. R. Westmoreland. "From quantum chemistry to kinetics via trajectory simulations, transition state theory, and the master equation." *Preprints, Division of Physical Chemistry*, Paper 538. 227th ACS National Meeting of ACS, Anaheim CA, March 28-April 1, 2004.
- 22nd Regional Meeting on Chemical Kinetics and Dynamics, Wadsworth Center, Albany NY, January 31, 2004.**
- P163. P.R. Westmoreland, S.I. Stoliarov, M.R. Nyden. "The Development of Reactive Molecular Dynamics for Modeling Polymers and Molecular Assemblies."
- P162. M.E. Law and P.R. Westmoreland, "Flame Kinetics from MBMS and Modeling."
- P161. A. Schoemann and P. R. Westmoreland, "Kinetics of Polymer Decomposition."
- Annual Meeting of AIChE, San Francisco CA, November 16-21, 2003:**
- P160. P.R. Westmoreland, S.I. Stoliarov, M.R. Nyden. "The Development of Reactive Molecular Dynamics for Modeling Polymers and Molecular Assemblies," Paper 560a.
- P159. S.I. Stoliarov, M.R. Nyden, R. E. Lyon, P.R. Westmoreland. "Application of Reactive Molecular Dynamics to the Study of the Thermal Degradation of Polyolefins," Paper 559a. **Invited.**
- Chemical and Physical Processes of Combustion, Fall Technical Meeting, Eastern Section of the Combustion Institute, State College PA, October 26-29, 2003:**
- P158. M. E. Law, A. Morel, P. R. Westmoreland, T. A. Cool, C. Taatjes. "Selective Detection of C₃H₄ and C₆H₆ Isomers in Flames," pp. 285-288.
- P157. A. Morel, M. E. Law, P. R. Westmoreland, T. A. Cool, K. Nakajima, T. A. Mostefaoui, F. Qi, A. Mcllroy, L. Poisson, D. S. Peterka, M. Ahmed. "Selective detection of isomers using a new photoionization MBMS apparatus," pp. 281-284.
- P156. A. Schoemann, P.R. Westmoreland, R. J. Farris, R. Kumar, A. C. Watterson, L. Samuelson. "New fire-safe polysiloxane polymers," pp. 49-52.
- P155. P.R. Westmoreland, H. Zhang, A. Schoemann, T. Inguilizian, R. J. Farris. "Developing fire-safe polymers using milligram-scale test methods," pp. 53-56.
- P154. A. Mcllroy, T. A. Cool, P. R. Westmoreland, and F. Qi. "Vacuum-ultraviolet photoionization probing of flame chemistry." Division of Physical Chemistry, Paper E-502. 225th ACS National Meeting, New Orleans LA, March 23-27, 2003.
- 3rd Joint Technical Meeting of the U.S. Sections of the Combustion Institute, Chicago IL, March 16-19, 2003:**
- P153. M.E. Law, G.E. Oulundsen III, P. R. Westmoreland, "Aromatic Ring Formation within Premixed Allene-Doped Ethylene Flat Flames," Paper F25.
- P152. S.J. Klippenstein, Y. Georgievskii, J.A. Miller, J.A. Nummela, B.K. Carpenter, P.R. Westmoreland, "Vinyl + O₂: A Complete Theoretical Treatment," Paper A39.
- Annual Meeting of AIChE, Indianapolis IN, November 3-8, 2002:**
- P151. M.E. Law, P.R. Westmoreland. "Modeling and New Data in Fuel-Lean Ethylene Flames," Paper 392b.
- P150. P.R. Westmoreland, M.R. Nyden, S.I. Stoliarov. "A Unified Reaction Rate Theory for Large Molecules in Condensed Phases," Paper 364b.
- P149. P.R. Westmoreland. "Developing Chemicals, Materials, and Processes through Computational Chemistry." AspenWorld 2002, Washington DC, October 28-31, 2002. **Invited.**
- P148. H. Zhang, P.R. Westmoreland, R.J. Farris, Division of Polymeric Materials: Science and Engineering, 224th National Meeting of ACS, Boston MA, August 18-22, 2002.
- P147. F. Qi, A. Mcllroy, T. A. Mostefaoui, T. A. Cool, P. R. Westmoreland, D. S. Peterka, L. Poisson, M. Ahmed, "A New Photoionization Molecular-Beam Mass Spectrometer for Low-Pressure Flame

- Structure Studies Using High-Intensity Synchrotron Radiation," Poster 024-3, 29th International Symposium on Combustion, Sapporo, Japan, July 21-26, 2002.
- P146. M.R. Nyden, S.I. Stoliarov, P.R. Westmoreland, C. Jee. "Applications of Reactive Molecular Dynamics to the Study of the Thermal Decomposition of Polymers and NanoScale Structures." International Conference on Multiscale Materials Modeling, Queen Mary University of London, June 17-20, 2002.
- P145. M.R. Nyden, S.I. Stoliarov, P.R. Westmoreland, Z. X. Guo, C. Jee. "Further Developments in Modeling the Thermal Decomposition of Polymers." 13th BCC Conference on Flame Retardancy, Stamford CT, June 3-5, 2002.
- 223rd National Meeting of ACS, Orlando, April 7-11, 2002:**
- P144. P.R. Westmoreland, S.I. Stoliarov, H. Zhang, M.R. Nyden. "Modeling and identifying intramolecular mechanisms of polymer degradation," Physical Chemistry Division, PHYS-516.
- P143. H. Zhang, E.B. Coughlin, P.R. Westmoreland, R.J. Farris, A. Plichta, Z.K. Brzozowski, "Fire-resistant, UV/Visible-sensitive polyarylates and copolymers," Division of Polymeric Materials: Science and Engineering, POLY-014.
- Chemical and Physical Processes of Combustion, Fall Technical Meeting, Eastern Section of the Combustion Institute, Hilton Head Island SC, December 2-5, 2001:**
- P142. T. Carrière, P.R. Westmoreland, "Complete Solution of the Flat-Flame Equations in the Non-Adiabatic Case," Paper 52, pp. 241-244.
- P141. M.E. Law, T. Carrière, P.R. Westmoreland, "New Insights into Fuel-Lean Ethylene Flames," Paper 40, pp. 194-197.
- Annual Meeting of AIChE, Reno NV, November 4-9, 2001:**
- P140. P. R. Westmoreland, T. Carrière, and M. Law. "Probing Pollutant Chemistry in Flames with MBMS and Modeling," Paper 362d.
- P139. S. I. Stoliarov, P. R. Westmoreland and M. R. Nyden. "Understanding Polymer Pyrolysis using a New Reactive Molecular Dynamics Method," Paper 361a.
- P138. P. R. Westmoreland, "Teaching about Kinetics and Molecular Simulations Using Web-Based Reactive Molecular Dynamics," Paper 2b.
- P137. P. R. Westmoreland and P. T. Cummings. "Uses of Computational Chemistry at Rohm and Haas: Some Case Studies," Paper 1c.
- Third Triennial International Fire & Cabin Safety Research Conference, Atlantic City, NJ, October 25-28, 2001:**
- P136. H. Zhang, P.R. Westmoreland, and R.J. Farris. "Thermal decomposition and combustion behavior of poly(hydroxyamide) (PHA) and its derivatives."
- P135. M.R. Nyden, G.P. Forney, S.I. Stoliarov, and P.R. Westmoreland. "New Reactive Molecular Dynamics Algorithm for Modeling the Thermal Decomposition of Polymers."
- P134. H. Zhang, P.R. Westmoreland, and R.J. Farris. "Thermal decomposition and combustion behavior of poly(hydroxyamide) (PHA) and its derivatives," 222nd National Meeting of ACS, Chicago, August 26-30, 2001, PMSE-277. *Proceedings of the ACS Division of Polymeric Materials: Science and Engineering*, **85**, 463-464 (2001).
- P133. P.R. Westmoreland, S.I. Stoliarov, and M.R. Nyden. "Reactive molecular dynamics of polymer decomposition using ab initio potential energy surfaces." 2nd International Workshop on Mesoscale Modeling, Brookline MA, August 13-14, 2001.
- New England Regional Meeting (NERM) of ACS, Univ. of New Hampshire, June 25-27, 2001:**
- P132. H. Zhang, P.R. Westmoreland, and R.J. Farris. "Thermal decomposition and combustion behavior of poly(hydroxyamide) and its derivatives."
- P131. H. Zhang, P.R. Westmoreland, and R.J. Farris. "Quantitative measurements on the flammability and thermal decomposition of polymers."
- P130. T. Carrière, P. R. Westmoreland, A. Kazakov, Y.S. Stein, and F.L. Dryer, "Modeling ethylene combustion from low to high pressure," 2nd Joint Technical Meeting of the U.S. Sections of the Combustion Institute, Oakland CA, March 25-28, 2001. *Proceedings of the Second Joint Technical Meeting of the U.S. Sections of the Combustion Institute*, The Combustion Institute: Pittsburgh, Paper 89 (2001).
- R129. P.R. Westmoreland. "International Activities in Computational Materials Science." *AMPTIAC Newsletter* **5**(1), 12-14 (2001).

- Annual Meeting of AIChE, Los Angeles CA, November 12-17, 2000:**
- P128. G. E. Oulundsen, T. Carrière, P. R. Westmoreland. "Molecular-Beam Mass Spectrometry and Modeling of an Ethylene Flame Doped with Allene" Paper 341a.
- P127. P. R. Westmoreland. "Chemistry and Life Sciences in a New Vision of Chemical Engineering," Paper 54c. **Invited.**
- 220th National Meeting of ACS, Washington DC, August 20-24, 2000.**
- P126. P. R. Westmoreland. "Complexity of kinetics and product channels for the reaction of vinyl reaction with oxygen," Paper PHYS-293, Symposium on "Industrial Applications of Theoretical Chemistry." **Invited.**
- P125. P. R. Westmoreland. "Predicting aromatics formation from propargyl reactions." Paper FUEL-5, Symposium on "1990 Clean Air Act Amendments: A Ten-Year Assessment." **Invited.**
- P124. T. Carrière, P. R. Westmoreland, "Temperature Profiles, Energy Balances, and the Modeling of MBMS Flame Data," 28th International Symposium on Combustion, Edinburgh Scotland, July 30-August 4, 2000. Poster 5-D18.
- P123. P. R. Westmoreland. "Combining Ab Initio Modeling with Experimental Kinetics to Develop New Polymers." "Solving Old Problems with New Methods - A Symposium on Computational Quantum Chemistry," New England Regional Meeting (NERM) of ACS, Univ. of Connecticut, June 20, 2000. **Invited.**
- P122. P. R. Westmoreland. "Combining Ab Initio Modeling with Experimental Kinetics to Develop New Polymers." CCLMS Conference on "Materials Design: Experimental and Computational Challenges," Baton Rouge LA, March 2-4, 2000. **Invited.**
- P121. P. R. Westmoreland and K. Rotem. "Polyhydroxyamide Pyrolysis Mechanism from Ab Initio Calculations," Annual Meeting of AIChE, Dallas TX, October 31-November 5, 1999. Paper 286b.
- P120. T. Carrière and P. R. Westmoreland, "Improving Kinetic Models for Ethylene Flat Flames," *Chemical and Physical Processes of Combustion*, Fall Technical Meeting, Eastern Section of the Combustion Institute, Raleigh NC, October 27-29, 1999, Paper 24, pp. 125-128.
- P119. P. R. Westmoreland, "A Fast Trip through the Methods of Computational Quantum Chemistry." The Catalysis Society of New England, Annual Spring Symposium, Worcester MA, May 1, 1999. **Invited.**
- 217th National Meeting of ACS, Anaheim CA, March 21-25, 1999.**
- P118. P. R. Westmoreland, K. Rotem, T. Ingulizian, C. Gao: S.W. Kantor, R.E. Lyon, "Developing polyhydroxyamide as a low-flammability polymer: An interplay among computational chemistry, polymer synthesis, and kinetics data," Paper COMP099. **Invited.**
- P117. M. R. Zachariah, D. Burgess, W. Tsang, P. R. Westmoreland, "Reaction engineering of flame suppression: Integrating ab initio computations into flow/chemistry modeling," Paper COMP062. **Invited.**
- P116. T. Carrière, A. Bhargava, and P. R. Westmoreland, "Sensitivity of the CO+OH rate constant in modeling a lean ethylene flame," 1st Joint Technical Meeting of the U.S. Sections of the Combustion Institute, Washington DC, March 15-17, 1999. *Proceedings of the First Joint Technical Meeting of the U.S. Sections of the Combustion Institute*, The Combustion Institute: Pittsburgh, 132-135 (1999).
- P115. P. R. Westmoreland, "A Course on 'Chemical Principles of Engineering.'" Symposium on Molecular Modeling in the Undergraduate Curriculum, Amherst MA, January 8, 1999.
- Annual Meeting of AIChE, Miami FL, November 15-19, 1998:**
- P114. P. R. Westmoreland, "A Course on 'Chemical Principles of Engineering'," Paper 54g.
- P113. P. R. Westmoreland, "Continuum Engineering Properties from the Schroedinger Equation," Paper 310f. **Invited.**
- P112. P. R. Westmoreland, "*Ab Initio* Quantum Chemistry: Case Studies," Paper 48e.
- P111. P. R. Westmoreland, "*Ab Initio* Quantum Chemistry: Thermochemistry and Kinetics," Paper 48a.
- P110. P. R. Westmoreland, "PECVD Kinetics from Probe Sampling," 194th Meeting of Electrochemical Society, Boston MA, November 1-6, 1998. Paper 797. **Invited.**
- P109. P. R. Westmoreland, "Extrapolating Growth Kinetics from the Gas to the Liquid Phase," Symposium on "The Structure of Jet Fuels," 216th National Meeting of ACS, Boston MA, August 23-27, 1998. *Preprints of Division of Petroleum Chemistry*, ACS, **43**(3), 442-444 (1998). **Invited.**
- 27th International Symposium on Combustion, Boulder CO, August 2-7, 1998.**
- P108. Anuj Bhargava, P. R. Westmoreland, "C₂H₄ Kinetics from Fuel-Rich and Fuel-Lean Ethylene Flames," Poster W2B06.

- P107. Anuj Bhargava, P. R. Westmoreland, "Impact of Improved Kinetics on Modeling of Ethylene Flames," Poster W2B05.
2nd Annual Green Chemistry and Engineering Conference, National Academy of Science, June 30-July 2, 1998:
- P106. P. R. Westmoreland, "Report from Workshop on 'The Role of Polymer Research in Green Chemistry and Engineering,' June 10-12, 1998."
- P105. P. R. Westmoreland, "Design, Synthesis, and Properties of Fire-Safe Polymers."
- P104. P. R. Westmoreland and S. V. Rao, "Using Quantum Chemistry for Technological Solutions," Connecticut Valley Quantum Chemistry Group, E. Hartford CT, April 8, 1998.
- P103. P. R. Westmoreland and A. Bhargava, "Kinetics of Formaldehyde and Formyl Reaction Pathways Measured in Ethylene Flames," Division of Physical Chemistry, 215th National Meeting of ACS, Dallas TX, March 29-April 4, 1998. Paper 229d. **Invited.**
- P102. S. V. Rao and P. R. Westmoreland, "Kinetics of NO_x-Generating H/N/O Reactions Through Theoretical Methods." Sixteenth Regional Meeting on Chemical Kinetics and Dynamics, Union College, Union NY, January 31, 1998.
- P101. P. A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Simulations of Flammability and Ignitability of Catalytic Oxidation Reactors with Detailed Reaction Mechanisms," Annual Meeting of AIChE, Los Angeles CA, November 16-21, 1997. Paper 273d.
Chemical and Physical Processes of Combustion, Fall Technical Meeting, Eastern Section of the Combustion Institute, Hartford CT, October 27-29, 1997:
- P100. P.-A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Self-Sustained Oscillations in Distributed Flames Modeled with Detailed Chemistry," Paper 14, pp. 201-204.
- P99. A. Bhargava and P. R. Westmoreland, "C₂H₄+H and C₂H₄+OH Chemistry Measured in Laminar, Premixed Flat Flames," Paper 89, pp. 337-340.
- P98. P. R. Westmoreland, "Assembling a Reaction Mechanism for CF₃CHFCF₃ in Flames," Symposium on Kinetic Modeling of Flame Suppression, Wright-Patterson Air Force Base, Dayton OH, July 15-17, 1997. **Invited.**
- P97. M. A. Tanoff, R. R. Dobbins, M. D. Smooke, D. R. Burgess, M. R. Zachariah, W. Tsang, and P. R. Westmoreland, "C₁ and C₂ Fluorinated Hydrocarbon Effects on the Extinction Characteristics of Methane vs. Air Counterflow Diffusion Flames," *Halon Options Technical Working Conference Proceedings*, pp. 116-127, Albuquerque NM, May 6-8, 1997.
Fifteenth Regional Meeting on Chemical Kinetics and Dynamics, Rensselaer Polytechnic Institute, Troy NY, January 25, 1997:
- P96. A. Bhargava and P. R. Westmoreland, "Measured Flame Structure and Kinetics in a Fuel-Rich Ethylene Flame."
- P95. K. Rotem and P. R. Westmoreland, "Calculating Thermochemistry and Kinetics of NO_x Using *Ab Initio* Methods."
Fall Technical Meeting, Eastern Section of the Combustion Institute, Hilton Head SC, December 9-11, 1996.
- P94. G. E. Oulundsen and P. R. Westmoreland, "Initial Measurements from Reacting Flows of Hydrocarbons with Chlorine," Paper 104.
- P93. A. Bhargava and P. R. Westmoreland, "MBMS Analysis of a Fuel-Lean Ethylene Flame," Paper 109.
Annual Meeting of AIChE, Chicago IL, November 10-15, 1996.
- P92. P. R. Westmoreland, "Bringing Molecular Modeling into the Chemical Engineering Curriculum," Paper 136a.
- P91. G. T. Linteris, D. R. Burgess, V. I. Babushok, M. R. Zachariah, W. Tsang, and P. R. Westmoreland, "Inhibition of Premixed Methane-Air Flames by Fluoromethanes and Fluoroethanes: Comparison between Flame Speed Measurements and Flame Structure Modeling Results," Paper 26i and Poster 122r.
- P90. A. Bhargava and P. R. Westmoreland, "Oxidation Chemistry Measured and Modeled in a Lean Ethylene Flames," Paper 58a.
- P89. J. W. Peterson and P. R. Westmoreland, "Time-Dependent Rate Coefficients for the Chemically Activated Dissociation of sec-Butyl Radical," Paper 131k.
- P88. P. A. Bui, D. G. Vlachos, and P. R. Westmoreland, "On the Self-Inhibition of Surface Fuel Ignition in Catalytic Oxidation Reactors," Paper 150b.

- P87. K. Rotem and P. R. Westmoreland, "Calculating Thermochemistry and Kinetics of NO_x Using *Ab Initio* Methods," Paper 199i.
- P86. P.-A. Bui, D. G. Vlachos, P. R. Westmoreland, "Simulations on catalytic ignition with detailed surface kinetics," Western States Section Meeting, Combustion Institute, Los Angeles CA, October 28-30, 1996.
- 26th International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996:**
- P85. P.-A. Bui, D. G. Vlachos, P. R. Westmoreland, "On the Self-Inhibition of Surface Fuel Ignition in Catalytic Oxidation Reactors," Poster P287.
- P84. Anuj Bhargava, P. R. Westmoreland, "Combustion Chemistry Measured in a Rich Ethylene Flame," Poster P43.
- P83. G. Skevis, P. Lindstedt, S. D. Thomas, A. Bhargava, and P. R. Westmoreland, "Modeling Propene Flames," 15th Journees d'Etudes of the Belgian Section of the Combustion Institute, Catholic University of Louvain, Louvain-la-Neuve Belgium, May 20-21, 1996.
- P82. P. A. Bui, D. G. Vlachos, and P. R. Westmoreland, "The Role of Platinum in Homogeneous Oxidation Chemistry," 1995 Fall Symposium, Catalysis Society of New England, Worcester MA, April 20, 1996.
- P81. P. R. Westmoreland, "Applications of Computational Quantum Chemistry in Chemical Engineering," Connecticut Valley Quantum Chemistry Group, Amherst MA, March 8, 1996.
- P80. M. A. Tanoff, R. R. Dobbins, M. D. Smooke, D. R. Burgess, M. R. Zachariah, W. Tsang, and P. R. Westmoreland, "C₁ Fluoro- and Hydrofluorocarbon Effects on the Extinction Characteristics of Methane vs. Air Counterflow Diffusion Flames," Sixth International Conference on Numerical Combustion, New Orleans LA, March 4-6, 1996.
- Fourteenth Regional Meeting on Chemical Kinetics and Dynamics, Amherst MA, January 27, 1996:**
- P79. P. A. Bui, I. B. Graff, D. G. Vlachos, and P. R. Westmoreland, "Extracting Kinetics from PECVD Experiments using Transport Analysis."
- P78. P. A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Kinetics and Bifurcations in Catalytic Combustion."
- P77. P. R. Westmoreland, "Applying Molecular and Materials Modeling for Chemical Engineering," Symposium on Molecular Modeling in the Undergraduate Curriculum, Department of Chemistry, University of Massachusetts Amherst, January 18, 1996.
- P76. E. Blunt-Harris, D. Boisclair, J. Clark, L. Craker, S. DiNardi, D. Hoagland, J. Meyer, P. Morgan, M. Rausch, D. Robinson, P. Samal, L. Schwartz, V. Steinberg, M. Weinberg, E. Westhead, and P. Westmoreland, *Laboratory Health and Safety Manual*, University of Massachusetts Amherst (1995).
- Annual Meeting of AIChE, Miami Beach FL, November 12-17, 1995:**
- P75. M. R. Zachariah, D. R. Burgess, and P. R. Westmoreland, "Understanding Trends in Bond Energy from Conformation Energy Effects and Mulliken Charge Population Analysis," Paper 53c.
- P74. P. A. Bui, I. B. Graff, D. G. Vlachos, and P. R. Westmoreland, "Measurement of Consumption and Generation Rates in a Plasma-Enhanced Chemical Vapor Deposition Reactor," Paper 157d.
- P73. P. R. Westmoreland, "Applying Molecular and Materials Modeling for Chemical Engineering," Research Computing Symposium, College of Natural Sciences and Mathematics, University of Massachusetts Amherst, October 27, 1995.
- Fall Technical Meeting, Eastern Section of the Combustion Institute, Worcester MA, October 16-18, 1995:**
- P72. M. A. Tanoff, R. R. Dobbins, M. D. Smooke, D. R. Burgess, M. R. Zachariah, W. Tsang, and P. R. Westmoreland, "Modeling Halon Flame Suppression in Diffusion Flames," pp. 451-454.
- P71. J. W. Peterson and P. R. Westmoreland, "Time-Dependent Solutions of the Master Equation for Chemically Activated Reactions," pp. 107-110.
- P70. P. A. Bui, D. G. Vlachos, and P. R. Westmoreland, "Inhibition of Homogeneous Ignition by a Catalytic Surface," pp. 147-150.
- P69. P.R. Westmoreland, "Vinyl-Oxygen Kinetics: A Reaction Engineering Problem Resolved with Computational Chemistry," Fifth Engineering Foundation Conference on Chemical Reaction Engineering, St. Augustine FL, October 8-13, 1995.

Thirteenth Regional Meeting on Chemical Kinetics and Dynamics, General Electric Corporate R&D Center, Schenectady NY, January 28, 1995:

- P68. G. E. Oulundsen and P. R. Westmoreland, "Exploring Hydrocarbon/Cl₂ Gas-Phase Reactions;"
- P67. J. W. Peterson and P. R. Westmoreland, "Time-Dependent Solutions of the Master Equation for Chemically Activated Reactions;"
- P66. I. B. Graff and P. R. Westmoreland, "Determination of Radical and Stable Species Concentrations in PECVD by Molecular-Beam Mass Spectrometry;"
- P65. Pierre Bui, D. G. Vlachos, and P. R. Westmoreland, "Data Analysis of Gas-Phase Neutrals in a PECVD Reactor."
- P64. P. R. Westmoreland and D. J. Hennessey, "On the Reaction of Vinyl with Oxygen," Paper 89, Fall Technical Meeting, Eastern Section of the Combustion Institute, Clearwater Beach FL, December 5-7, 1994, pp. 425-428.

Annual Meeting of AIChE, San Francisco CA, November 13-19, 1994:

- P63. I. Bradford Graff and P. R. Westmoreland, "Determination of Radical and Stable Species Concentrations in PECVD by Molecular-Beam Mass Spectrometry," Paper 4b.
- P62. M. R. Zachariah, P. R. Westmoreland, D. Burgess Jr., W. Tsang, C. F. Melius. "Application of Bond Additivity Corrected-MP4 to the Calculation of Thermochemical and Kinetic Properties of Fluorocarbons," Paper 64e.
- P61. W. Shi and P. R. Westmoreland, "Molecular-Scale Modeling of Steam Cracking of Propane," Paper 64f.
- P60. P. R. Westmoreland, "Modeling the Lean Combustion of Propylene," Paper 74f.
- P59. P. R. Westmoreland, Scott D. Thomas, and Anuj Bhargava, "Obtaining Kinetics from MBMS and Modeling of Propene Flame Structure," Specialists Workshop on Applications of Free-Jet, Molecular-Beam, Mass Spectrometric Sampling; Estes Park CO, October 12-14, 1994; Publication NREL-CP-433-7748, National Renewable Energy Laboratory, pp. 110-115 (1994).

208th National Meeting of ACS, Washington DC, August 21-26, 1994:

- P58. M. R. Zachariah, P. R. Westmoreland, W. Tsang, and D. R. F. Burgess, Jr., "Theoretical Prediction of Thermochemistry and Kinetics of Fluorocarbons," Preprints of Div. of Environmental Chemistry, American Chemical Society, 34(2), 771.
- P57. D. R. F. Burgess, Jr., P. R. Westmoreland, W. Tsang, M. R. Zachariah, A. W. Miziolek, R. G. Daniel, and K. L. McNesby, "Key Species and Important Reactions in Fluorinated Hydrocarbon Flame Chemistry: Premixed Flame Simulations and Measurements," Preprints of Div. of Environmental Chemistry, American Chemical Society, 34(2), 776-780.

Twenty-Fifth Symposium (International) on Combustion, Irvine CA, July 31-August 5, 1994:

- P56. S. D. Thomas and P. R. Westmoreland, "Allyl Oxidation Chemistry in a Lean Propene Flame," Work-in-Progress Poster 3-96.
- P55. A. W. Miziolek, R. G. Daniel, K. L. McNesby, W. Tsang, V. Babushok, M. R. Zachariah, P. R. Westmoreland, D. R. F. Burgess, Jr., "Tunable Diode Laser and Modeling Flame Structure Studies of Inhibited 20-Torr Flames," Work-in-Progress Poster 4-20.
- P54. A. W. Miziolek, A. J. Finnerty, R. G. Daniel, K. L. McNesby, W. Tsang, V. Babushok, M. R. Zachariah, P. R. Westmoreland, D. R. F. Burgess, Jr., "Fundamental Studies of Fire Extinguishment for Predicting Halon Alternative Compound Development," Army Research Conference, Orlando FL, June 21-24, 1994.

Halon Options Technical Working Conference, Albuquerque NM, May 3-5, 1994:

- P53. D. R. F. Burgess, Jr., W. Tsang, M. R. Zachariah, P. R. Westmoreland, "Kinetics of Fluorine-Inhibited Hydrocarbon Flames," pp. 489-500.
- P52. R. G. Daniel, K. L. McNesby, A. W. Miziolek, D. R. F. Burgess, Jr., P. R. Westmoreland, W. Tsang, M. R. Zachariah. "IR Laser Absorption and Modeling Studies of Hydrocarbon Flames Inhibited by Candidate Halon Replacement Compounds," pp. 229-239.
- P51. D. Burgess, Jr., W. Tsang, M. R. Zachariah, P. R. Westmoreland, "Fluorinated Hydrocarbon Flame Suppression Chemistry," Preprints of Div. of Fuel Chemistry, American Chemical Society, **39**, No. 1, 141-146 (1993); presented at the 207th National Meeting of ACS, San Diego CA, March 13-19, 1994.
- P50. I. B. Graff, R.A. Pugliese, Jr., P. R. Westmoreland, "Mapping Chemistry and Transport in PECVD of Diamondlike Carbon," Paper W1.19, Materials Research Society, 1993 Fall Meeting, Boston MA, November 29-December 3, 1993.

1993 Annual Meeting of AIChE, St. Louis MO, November 7-12, 1993:

- P49. I. B. Graff, P. R. Westmoreland, "Mapping Concentration Data in PECVD of Diamond-like Carbon," Paper 95c.
- P48. P. R. Westmoreland, "Obtaining the Mechanism for Lean Propylene Combustion from a Detailed Reaction Set," Paper 20b, 1993 Annual Meeting of AIChE, St. Louis MO, November 7-12, 1993.
- P47. D. R. F. Burgess, Jr., W. Tsang, P. R. Westmoreland, M. R. Zachariah, "Chemistry of Fluorinated Species in Hydrocarbon Flames," Paper 25d.
- P46. P. R. Westmoreland, D. R. F. Burgess, Jr., W. Tsang, M. R. Zachariah, "Kinetics of Fluoromethanes in Flames," Paper 108, Fall Technical Meeting, Eastern States Section of the Combustion Institute, Princeton NJ, October 25-27, 1993, pp. 479-482.
- P45. D. Burgess, W. Tsang, P.R. Westmoreland, M.R. Zachariah, "Chemistry of Halon Fire Suppressants," International Conference on Chemical Kinetics, National Institute of Standards and Technology, July 12-16, 1993, p. 71.
- P44. P.R. Westmoreland, "Getting Reactions and Mechanisms from Experiments Integrated with Computational Chemistry," Invited lecture, Fourth Engineering Foundation Conference on Chemical Reaction Engineering, Palm Coast FL, February 21-26, 1993.

1992 Annual Meeting of AIChE, Miami Beach FL, November 1-6, 1992.

- P43. R.A. Pugliese, Jr., P.R. Westmoreland, "Kinetics of Electron-Impact Dissociation of Methane in PECVD of Diamondlike Carbon," Paper 197i.
- P42. P.R. Westmoreland, "Kinetics of Allyl Radical," Paper 54e.
- P41. P.R. Westmoreland, "Predicting Kinetics for $\text{SiH}_3 + \text{O}_3$," SEMATECH/NIST Workshop on Chemistry of CVD Processes in Semiconductor Manufacturing, Gaithersburg MD, September 29-30, 1992.

24th International Symposium on Combustion, Sydney, Australia, July 5-10, 1992.

- P40. P.R. Westmoreland, "Kinetics of the Vinyl + Oxygen Reaction," Poster P55, 24th International Symposium on Combustion, Sydney, Australia, July 5-10, 1992.
- P39. M.G. Michaud and P.R. Westmoreland, "Testing an Improved Flame Mechanism for Oxidation and NO_x Kinetics," Poster P184.
- P38. P.R. Westmoreland, " C_3H_3 Reaction Kinetics in Fuel-Rich Flames," Tenth Regional Meeting on Chemical Kinetics and Dynamics, Rensselaer Polytechnic Institute, Troy NY, February 1, 1992.
- P37. R.A. Pugliese, Jr., P.R. Westmoreland, "Microprobe Measurements in PECVD of Diamondlike Carbon," Paper 27i, 1991 Annual Meeting of AIChE, Los Angeles CA, November 17-22, 1991.
- P36. S.D. Thomas, F. Communal, P.R. Westmoreland, " C_3H_3 Reaction Kinetics in Fuel-Rich Flames," Preprints of Div. of Fuel Chemistry, American Chemical Society, **36**, No. 4, 1448-1455 (1991); presented at the Symposium on Combustion Chemistry, 202nd National Meeting of ACS, New York NY, August 25-30, 1991.

Ninth Regional Meeting on Chemical Kinetics and Dynamics, Skidmore College, Saratoga Springs NY, January 19, 1991.

- P35. P.R. Westmoreland, "Developing Master-Equation Methods for Engineering Kinetics."
- P34. S.D. Thomas and P.R. Westmoreland, "Molecular-Beam Mass Spectrometry in Flames: Verification of an Ethene Mechanistic Model."
- P33. R.A. Pugliese, Jr., and P.R. Westmoreland, "Reaction Kinetics in PECVD Kinetics of Amorphous Silicon: Experiments and Mechanistic Modelling."
- P32. Wen Shi and P.R. Westmoreland, "Steam Cracking Mechanisms."

1990 Annual Meeting of AIChE, Chicago, November 11-16, 1990.

- P31. P.R. Westmoreland, "Developing Master-Equation Methods for Engineering Kinetics," Paper 54c.
- P30. S.D. Thomas and P.R. Westmoreland, "Kinetics of Ethylene Combustion from Flat-Flame Modeling," Paper 119d.
- P29. F. Communal and P.R. Westmoreland, "Predicted Kinetics for $\text{SiH}_2 + \text{O}_2$: Association with Multiple Isomerizations," Paper 140f.
- P28. F. Communal and P.R. Westmoreland, "Predicted Kinetics for $\text{SiH}_2 + \text{O}_2$: Association with Multiple Isomerizations," Paper 98, Fall Technical Meeting, Eastern Section of the Combustion Institute, Orlando FL, December 3-5, 1990.
- P27. F. Communal, S.D. Thomas, and P.R. Westmoreland, "Kinetics of C_3 Routes to Aromatics Formation," Poster P40, 23rd International Symposium on Combustion, Orléans, July 22-27, 1990.

1989 Annual Meeting of AIChE, San Francisco CA, November 5-10, 1989:

- P26. S.D. Thomas and P.R. Westmoreland, "Role of C₃H₃ in Aromatics and Soot Formation," Paper 130g.
- P25. R.A. Pugliese, Jr., and P.R. Westmoreland, "Electronic Attachment and Electron Excitation in PECVD Kinetics," Paper 223f.

Fall Technical Meeting, Eastern Section of the Combustion Institute, Albany NY, Oct. 30-Nov. 1, 1989:

- P24. S.D. Thomas and P.R. Westmoreland, "Testing Predictions of C₂₋₄ Species in a Fuel-Rich Acetylene Flame," Paper 13.
- P23. P.R. Westmoreland, "On the Kinetics and Thermodynamics of C₄H₅ Isomers," Paper 15.
- P22. P.R. Westmoreland, "Analysis of C₄H₅ Chemistry for Aromatics Formation," Poster E-8, 2nd International Symposium on Chemical Kinetics, Gaithersburg MD, July 23-27, 1989.
- P21. P.R. Westmoreland, "The Importance of Obvious and Disguised Association Reactions in Combustion," Paper 17, Fall Technical Meeting, Eastern Section of the Combustion Institute, Clearwater Beach FL, December 5-7, 1988.

1988 Annual Meeting of AIChE, Washington DC, November 28-December 2, 1988:

- P20. P.R. Westmoreland, "Formation Reactions for Aromatics from Steam Cracking," Paper 167g.
- P19. R.A. Pugliese, Jr., and P.R. Westmoreland, "PECVD Modeling with Predicted Rate Constants," Paper 38a.
- P18. P.R. Westmoreland, "Analysis of C₄ Chemistry for Aromatics Formation and Destruction," Poster 147, 22nd International Symposium on Combustion, Seattle, August 14-19, 1988.
- P17. P.R. Westmoreland, "Development of Large Chemical Mechanisms for Combustion," Paper 27b, 1987 Annual Meeting of AIChE, New York, November 15-20, 1987.
- P16. P.R. Westmoreland, "Prediction of Kinetics for C₄ Species Which Form Benzene," Preprints of Div. of Fuel Chemistry, American Chemical Society, **32**, No. 3, 480 (1987); presented at the 194th ACS National Meeting, New Orleans, August 30-September 4, 1987.
- P15. P.R. Westmoreland, A.M. Dean, J.B. Howard, and J.P. Longwell, "Benzene Formation by Chemically Activated Isomerization," Paper 44, Fall Technical Meeting, Eastern Section of the Combustion Institute, San Juan, Puerto Rico, December 15-17, 1986.
- P14. P.R. Westmoreland, A.M. Dean, J.B. Howard, and J.P. Longwell, "Bimolecular QRRK as a Predictive Tool for Combustion Kinetics," Poster 106, 21st International Symposium on Combustion, Munich, August 3-8, 1986.
- P13. P.R. Westmoreland, J.B. Howard, and J.P. Longwell, "Analysis of Multiple Decompositions in Chemically Activated Reactions," Poster 118, Ninth International Symposium on Gas Kinetics, Bordeaux, July 20-25, 1986.
- P12. P.R. Westmoreland, J.B. Howard, J.P. Longwell, and A.M. Dean, "Pressure Effects on Rate Constants in Combustion and Pyrolysis," 1985 Annual Meeting of AIChE, Chicago, November 10-15, 1985.
- P11. P.R. Westmoreland, J.B. Howard, J.P. Longwell, and A.M. Dean, "Bimolecular QRRK as a Tool for Combustion Modeling," Paper 66, Fall Technical Meeting, Eastern Section of the Combustion Institute, Philadelphia, November 4-6, 1985.
- P10. P.R. Westmoreland, J.B. Howard, J.P. Longwell, and A.M. Dean, "Application of Quantum-RRK Methods to Combustion Reactions," 190th ACS National Meeting, Chicago, September 8-13, 1985.
- P9. L.S. Dickerson and P.R. Westmoreland, "Laboratory Studies Supporting In Situ Gasification," 73rd Annual Meeting of AIChE, Chicago, November 16-20, 1980.
- P8. R.W. Lyczkowski and P.R. Westmoreland, "The Role of Drying in Underground Coal Conversion Processes: A State-of-the-Art Review," Keynote Lecture at 2nd International Symposium on Drying, Montreal, Canada, July 6-9, 1980.
- P7. P.R. Westmoreland, "Measurement of Thermal Diffusivity and Application to In Situ Coal Gasification," *Proceedings of the 14th Intersociety Energy Conversion Engineering Conference*, Boston, August 5-10, 1979 (1979).
- P6. P.R. Westmoreland and L.S. Dickerson, "A Review of Supporting Research at ORNL for Underground Coal Gasification," *Proceedings of the 5th Underground Coal Conversion Symposium*, Alexandria (VA), June 18-21, 1979, U.S. Dept. of Energy, CONF-790630 (1979).
- P5. P.R. Westmoreland and L.S. Dickerson, "Pyrolysis of Blocks of Texas Lignite," 86th National Meeting of AIChE, Houston, April 1-5, 1979.

- P4. P.R. Westmoreland, "Pyrolysis of Bituminous Coal Blocks," *Proceedings of the 4th Underground Coal Conversion Symposium*, Steamboat Springs (CO), July 17-20, 1978, Sandia Laboratories, SAND 78-0941 (1978).
- P3. P.R. Westmoreland and R.C. Forrester, "Pyrolysis of Coal Blocks: Implications of Heat and Mass Transport Effects for In Situ Gasification," Preprints of Div. of Fuel Chemistry, American Chemical Society, **22** (1), 93 (1977); 173rd ACS National Meeting, New Orleans, March 21-25, 1977.
- P2. R.C. Forrester and P.R. Westmoreland, "Two-Dimensional Pyrolysis Effects during In Situ Coal Gasification: Preliminary Results," Paper SPE-6150, 51st Annual Fall Technical Conference and Exhibition of the Society of Petroleum Engineers of AIME, New Orleans, Oct. 3-6, 1976.
- P1. P.R. Westmoreland, "Coal Pyrolysis in Underground Coal Gasification," 11th Southeastern Seminar on Thermal Sciences, University of Tennessee at Knoxville, April 28-29, 1975.

II.E. Invited seminars (134)

II.E.1. Academic seminars (104)

- 2024 City University of New York, Department of Chemical Engineering, New York, NY.
- 2023 Missouri University of Science and Technology, Department of Chemical and Biochemical Engineering, Rolla MO.
- 2022 Dawood University of Engineering and Technology, Department of Chemical Engineering, Karachi, Sindh, Pakistan.
- 2022 Federal University of Rio de Janeiro, Department of Chemical Engineering, Termodinâmica Aplicado e Simulação Molecular, Brazil.
- 2022 University of Nevada Reno, Department of Chemical & Materials Engineering, Reno NV.
- 2022 Appalachian State University, Department of Chemistry, Boone NC.
- 2021 University of California Irvine, Mechanical and Aerospace Engineering, Irvine CA.
- 2018 University of Texas Permian Basin, College of Engineering, Odessa TX.
- 2018 Huazhong University of Science and Technology, Wuhan, China.
- 2018 Beihang University and North China Electric Power University (Joint seminar), Beijing, China.
- 2018 Columbia University, Department of Chemical Engineering, New York NY.
- 2017 Auburn University, Department of Chemical Engineering, Auburn AL.
- 2016 Zhengzhou University, Department of Chemical Engineering, Zhengzhou, China.
- 2016 Politecnico di Milano, Chemistry, Material and Chemical Engineering Department "Giulio Natta," Milan, Italy.
- 2016 Ashton University, Department of Chemical Engineering, Birmingham UK.
- 2016 Cambridge University, Gonville & Caius College, Chemical Engineering, Cambridge, UK.
- 2016 National University of Ireland, Galway IE.
- 2016 Oxford University, Chemical Engineering, Oxford, UK.
- 2016 Leeds University, Chemical Engineering, Leeds, UK.
- 2016 Ghent University, Chemical Engineering, Ghent, Belgium.
- 2016 University College London, Chemical Engineering, London, UK.
- 2016 Imperial College London, Chemical Engineering Leverhulme Lecture, London, UK.
- 2016 Imperial College London, Mechanical Engineering Distinguished Lecture, London, UK.
- 2016 University of Edinburgh, School of Engineering, Edinburgh, UK.
- 2015 Newcastle University, Department of Chemical Engineering, Newcastle upon Tyne, UK.
- 2015 Universität Duisburg-Essen, Faculty of Engineering, Duisburg, Germany.
- 2015 Université de Lorraine, École Nationale Supérieure des Industries Chimiques, Nancy, France.
- 2014 National Technical University of Athens, Department of Chemical Engineering, Athens, Greece.
- 2014 University of Canterbury, Department of Chemical Engineering, "Sanderson CAPE Prestige Seminar," Christchurch, New Zealand.
- 2014 University of California Los Angeles, Department of Chemical and Biomolecular Engineering, Los Angeles, CA.
- 2013 Peking University, Center for Water Research and College of Engineering, Beijing, China.
- 2013 Tsinghua University, Department of Chemical and Biomolecular Engineering, Beijing, China.
- 2013 Tianjin University, School of Chemical Engineering & Technology, Tianjin, China.
- 2013 Zhejiang University, Department of Chemical and Biological Engineering, Hangzhou, China.

- 2013 Nanjing University of Technology, Department of Chemical Engineering and State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing, China.
- 2013 Hong Kong University of Science and Technology, Department of Chemical and Biomolecular Engineering, Hong Kong, China.
- 2013 City University of New York, Department of Chemical Engineering, New York, NY.
- 2010 Case Western Reserve University, Department of Chemical Engineering, Cleveland, OH.
- 2010 Rice University, Department of Chemical Engineering, Houston, TX.
- 2010 University of Pittsburgh, Center for Modeling and Simulation, Pittsburgh PA.
- 2010 University of Pittsburgh, Department of Chemical and Petroleum Engineering, Pittsburgh PA.
- 2010 North Carolina State University, Department of Material Science and Engineering, Raleigh NC.
- 2009 University of Texas, Austin, Institute for Computational Engineering and Sciences, Austin, TX.
- 2009 Texas Tech University, Department of Chemical Engineering, Lubbock, TX.
- 2009 University of Tennessee, Department of Chemical Engineering, Knoxville TN.
- 2009 Tennessee Technological University, Department of Chemical Engineering, Cookeville, TN.
- 2009 University of Utah, Department of Chemical Engineering, Salt Lake City UT.
- 2008 North Carolina State University, Department of Chemical Engineering, Raleigh NC.
- 2008 Colorado School of Mines, Department of Chemical and Petroleum Engineering, Golden CO.
- 2008 University of Connecticut, Department of Mechanical Engineering, Storrs CT.
- 2007 George Washington University, Department of Chemistry, Washington DC.
- 2007 University of Kentucky, Department of Chemical and Materials Engineering, Lexington KY.
- 2005 University of Maryland, Department of Chemical and Biomolecular Engineering, College Park MD.
- 2005 New Jersey Institute of Technology, Department of Chemical Engineering, Newark NJ.
- 2005 Virginia Tech, Department of Chemical Engineering, Blacksburg VA.
- 2005 Vanderbilt University, Department of Chemical Engineering, Nashville TN.
- 2004 University of Arizona, Department of Chemical and Environmental Engineering, Tucson AZ.
- 2004 University of Rhode Island, Department of Chemical Engineering, Kingston RI.
- 2004 University of Pennsylvania, Department of Chemical and Biomolecular Engineering, Philadelphia PA.
- 2003 Purdue University, School of Chemical Engineering, W Lafayette IN.
- 2003 University of Texas, Department of Chemical Engineering, Austin TX.
- 2002 Massachusetts Institute of Technology, Department of Chemical Engineering, Cambridge MA.
- 2002 University of Delaware, Department of Chemical Engineering, Newark DE.
- 2002 New Mexico State University, Department of Chemical Engineering, Las Cruces NM.
- 2001 State University of New York, Department of Chemical Engineering, Buffalo NY.
- 2000 Texas A&M University, Department of Chemical Engineering, College Station TX.
- 2000 University of South Carolina, Department of Chemical Engineering, Columbia SC.
- 2000 Case Western Reserve University, Department of Chemical Engineering, Cleveland OH.
- 2000 University of Michigan, Department of Chemical Engineering, Ann Arbor MI.
- 2000 Tufts University, Department of Chemical Engineering, Medford MA.
- 1999 North Carolina State University, Department of Chemical Engineering, Raleigh NC.
- 1999 University of Minnesota, Department of Mechanical Engineering, Minneapolis MN.
- 1998 Brigham Young University, Department of Chemical Engineering, Provo UT.
- 1998 University of Utah, Department of Chemical Engineering, Salt Lake City UT.
- 1998 University of Minnesota, Dept of Chemical Engineering and Materials Science, Minneapolis MN.
- 1998 University of Connecticut, Department of Chemical Engineering, Storrs CT.
- 1997 University of Virginia, Department of Chemical Engineering, Charlottesville VA.
- 1997 Wesleyan University, Department of Chemistry, Middletown CT.
- 1997 University of Colorado, Department of Chemical Engineering, Boulder CO.
- 1997 Colorado School of Mines, Department of Chemical and Petroleum Engineering, Golden CO.
- 1996 University of North Carolina, Department of Chemistry, Chapel Hill NC.
- 1995 University of Massachusetts Computing Symposium, Amherst MA.
- 1995 Northwestern University, Department of Chemical Engineering, Evanston IL.
- 1995 Massachusetts Institute of Technology, Department of Chemical Engineering, Cambridge MA.
- 1995 University of Michigan, Department of Chemical Engineering, Ann Arbor MI.
- 1994 Princeton University, Department of Mechanical and Aerospace Engineering, Princeton NJ.
- 1994 Yale University, Department of Chemical Engineering, New Haven CT.
- 1993 University of Maryland, Department of Chemical Engineering, College Park MD.

- 1993 Pennsylvania State University, Department of Materials Science and Engineering, State College PA.
- 1992 State University of New York, Department of Chemical Engineering, Buffalo NY.
- 1992 Carnegie-Mellon University, Department of Chemical Engineering, Pittsburgh PA.
- 1991 New Jersey Institute of Technology, Department of Chemical Engineering, Chemistry, and Environmental Science, Newark NJ.
- 1991 George Washington University, Department of Chemistry, Washington DC.
- 1990 Worcester Polytechnic Institute, Department of Chemical Engineering, Worcester MA.
- 1990 University of Florida, Department of Chemical Engineering, Gainesville FL.
- 1990 Rensselaer Polytechnic Institute, Department of Chemical Engineering, Troy NY.
- 1990 University of Delaware, Department of Chemical Engineering, Newark DE.
- 1989 Western New England College, Springfield MA.
- 1988 Yale University, Department of Chemical Engineering, New Haven CT.
- 1987 University of Massachusetts Amherst, Department of Chemistry, Amherst MA.
- 1980 Virginia Polytechnic Institute, Department of Chemical Engineering, Blacksburg VA.
- 1979 University of New Hampshire, Department of Chemical Engineering, Durham NH.
- 1978 Tennessee Technological University, Department of Chemical Engineering, Cookeville TN.
- 1975 Tennessee Technological University, Department of Chemical Engineering, Cookeville TN.

II.E.2. Industrial, government, and other external seminars (33)

- 2023 Academy of Chemical Engineers Lecture, Missouri University of Science and Technology, Rolla MO.
- 2019 Science Heritage Institute, Philadelphia PA.
- 2018 Savannah River National Laboratory, Aiken SC.
- 2014, 2017 Eastman Chemical, Kingsport TN.
- 2009 National Academy of Science, Chemical Sciences Roundtable.
- 2008 Soldier Systems Center, U.S. Army, Natick MA.
- 2008 United Technologies Research Center, East Hartford CT.
- 2006 Air Force Office of Scientific Research, Space Propulsion Systems, Annapolis MD.
- 2005 US Environmental Protection Agency, Research Triangle Park NC.
- 2003 Philip Morris, Richmond VA.
- 2001 BP Research Center, Naperville IL.
- 2000 Lubrizol, Wickliffe OH.
- 1997 Spectran Inc., Sturbridge MA.
- 1996 United Technologies Research Center, E. Hartford CT.
- 1996 NRL Chemistry Colloquium Speaker, Naval Research Laboratory, Washington DC.
- 1994 E. I. Du Pont de Nemours and Company, Jackson Laboratory, Deepwater NJ.
- 1994 U. S. Army Research Laboratory, Aberdeen Proving Ground MD.
- 1994 ARCO Chemical Company, Newtown Square PA.
- 1994 Dow Chemical Company, Central Research, Midland MI.
- 1993 National Institute of Standards and Technology, Gaithersburg MD.
- 1993 Dow Chemical Company, Freeport TX.
- 1993 Naval Research Laboratory, Washington DC.
- 1992 Washington Area Discussion Group on the Chemical Physics of Small Molecules and Free Radicals, Washington DC.
- 1992 General Electric Company, Corporate Research and Development, Schenectady NY.
- 1991 National Institute of Standards and Technology, Gaithersburg MD.
- 1991 Digital Equipment Corporation, Hudson MA.
- 1991 E. I. Du Pont de Nemours and Company, Central Research and Development, Wilmington DE.
- 1990 Dow Chemical Company, Central Research, Midland MI.
- 1990 General Electric Company, Corporate Research and Development, Schenectady NY.
- 1990 Sandia National Laboratories, Combustion Research Facility, Livermore CA.
- 1988 General Electric Company, Corporate Research and Development, Schenectady NY.
- 1987 United Technologies Research Center, E. Hartford CT.

II.F. Financial grants awarded, including financial grants for equipment

II.F.1. Proposals under consideration

II.F.2. Active grants and contracts (by reverse chronological order of starting date)

U.S. Environmental Protection Agency.

"Predictive Chemical Models for Incineration of Novichok Agents," \$249,999, two years. Award period: 1/1/2025 - 12/31/2026.

U.S. Department of Defense.

"MURI: Combustion of Solid Fuels in High Enthalpy Flow," \$1,058,573 of \$7,500,000, five years. Co-PI with Gregory Young (Lead PI, Virginia Tech), James Michael (Iowa State), Suresh Menon (Georgia Tech), Hai Wang (Stanford), Richard Yetter (Penn State), Michael Zachariah (UC Riverside). Award period 6/1/2023 - 5/31/2028.

National Science Foundation ACCESS.

"Thermal Destruction Chemistry of Hazardous Substances" (Project CHE250144). Awarded Resources: 200,000.0 ACCESS Credits, 2025-08-13 to 2026-08-12.

II.F.3. Completed grants and contracts (chronological order)

U.S. Bureau of Mines.

Memorandum of Agreement No. 14-09-0050-3363, Long-term loan of flame MBMS apparatus and ancillary equipment, 1986.

National Science Foundation.

"Engineering Research Equipment Grant: Plasma-Enhanced Chemical Vapor Deposition Reactor" (Grant No. CBT-88-05703), \$26,000 plus \$13,000 matching funds from university, 5/1/88-10/31/90.

University of Massachusetts.

"Faculty Research Grant: Fundamental Chemistry of Steam Cracking," \$5,000, 6/1/88-10/31/89.

National Science Foundation.

"Research Initiation: Mapping Process Chemistry for Silicon PECVD" (Grant No. CTS-88-10562), \$70,000 plus \$10,000 matching funds from university, 7/1/88-6/30/90.

U.S. Department of Energy.

"Gas Chromatograph" (Agreement No. DOE-CH-30-90, "Energy-Related Laboratory Equipment Grants"), equipment with appraised value of \$1,963, February 1990.

U.S. Department of Energy.

"Preamplifier with Oscilloscope" (Grant No. DE-FG06-90R11909, "Energy-Related Laboratory Equipment Grants"), equipment with appraised value of \$2,617, March 1990.

United Technologies Research Center.

"Electropneumatically Actuated Vacuum Gate Valve, MDC Vacuum Products Corporation Model GV6000VP", used equipment with purchase value of \$2,075, March 1990.

Monsanto Chemical Company.

"Gas Chromatographs", used equipment, May 1990.

Digital Equipment Corporation.

"100% Allowance for Purchase of DEC Equipment and/or Software Licenses" (Grant No. 1079), \$45,750, 5/29/90-11/25/90.

National Science Foundation.

"Presidential Young Investigator Award" (Grant No. CTS-90-57406), \$312,500 including \$187,500 NSF match of industrial grants; 7/1/90-6/30/95.

U.S. Department of Energy.

"Photon Counter" (Grant No. AL-90-15, "Energy-Related Laboratory Equipment Grants"2), equipment with appraised value of \$2,995, August 1990.

Exxon Education Foundation.

"Molecular-Beam Mass Spectrometry of Reactive Intermediates" (Grant No. 13800), \$10,000, 9/1/90-8/31/91.

General Electric Corporate Research and Development.

"Combustion and Reaction Engineering Chemistry," \$20,000, 9/15/90-5/30/91.

General Electric Corporate Research and Development.

"Pressure Dependence of Gas-Phase Combustion Reactions," \$14,800, 6/1/91-10/31/91.

U.S. Department of Energy.

"Probing Flame Chemistry with MBMS, Theory, and Modeling" (Grant No. DE-FG02-91ER14192) \$242,000, 7/15/91-7/14/94.

Rohm and Haas Corporation.

Unrestricted grant, \$5,000, 8/1/91.

Exxon Education Foundation.

"Molecular-Beam Mass Spectrometry of Reactive Intermediates" (Grant No. 14023), \$15,000, 9/1/91-8/31/92.

General Electric Corporate Research and Development.

"Modeling of NO_x Combustion Reactions," \$20,000, 6/1/92-1/30/93.

National Institute of Standards and Technology.

"Interagency Personnel Agreement," (Grant No. IP2004), \$39,017, 9/1/92-8/30/93.

Dow Chemical Company.

"Fundamental Kinetics of Hydrocarbon/Chlorine Flames" (Dow Agreement No. 921575), \$53,000, 10/1/92-9/30/93.

E. I. du Pont, Engineering Experiment Station.

"Hewlett-Packard Gas Chromatograph", used equipment, January 1993.

Autodesk, Inc.

"Hyperchem", molecular modeling software, valuation \$3,500, April 1993.

Exxon Research and Engineering.

"Electronics for Extranuclear Laboratories Quadrupole Mass Spectrometer", used equipment, August 1993.

Dow Chemical Company.

"Fundamental Kinetics of Hydrocarbon/Chlorine Flames" (Dow Agreement No. 921575), \$57,000, 10/1/93-9/30/94.

University of Massachusetts Amherst.

"Faculty Research Grant: Applying Computational Chemistry in Chemical Engineering," \$5,000, 12/1/93-11/30/94.

National Institute of Standards and Technology.

"Interagency Personnel Agreement," (Grant No. IP4021), \$9,132, 6/19/94-7/30/94.

Dow Chemical Company.

Unrestricted grant in "Fundamental Kinetics of Hydrocarbon/Chlorine Flames," \$41,750, 10/1/94.

National Science Foundation.

"Engineering Research Equipment: A Computer Graphics Facility for Research in Applied Molecular and Materials Modeling" (Grant No. CTS-94-10994 with P.A. Monson, M. R. Cook, D. G. Vlachos), \$40,000 plus \$38,000 matching funds from university, 10/1/94-9/30/95.

U.S. Department of Energy.

"Probing Flame Chemistry with MBMS, Theory, and Modeling" (Grant No. DE-FG02-91ER14192, renewal) \$267,000, 1/1/95-6/30/98.

Dow Chemical Company.

Unrestricted grant in "Fundamental Kinetics of Hydrocarbon/Chlorine Flames," \$41,750, 10/1/95.

National Environmental Technology for Waste Reduction Institute (NETI).

"Kinetics for Controlling NO_x at the Source," \$49,000, 7/1/96-6/30/97.

Hewlett-Packard, Corvallis OR.

"KF vacuum valves", valuation \$1,500, April 1996.

U.S. Federal Aviation Administration and CUMIRP Cluster F (nine industrial participants).

"Research Program on High-Performance Fire-Safe Polymeric Materials," \$2,426,472 (P.I.: Richard Farris; Co-P.I.'s: Simon Kantor, Alan Lesser, Thomas McCarthy, William MacKnight, Bruce Novak, Phillip R. Westmoreland, 1994-1999; \$87,653 for PRW projects in 7/1/96-6/30/97; \$90,000 for PRW projects in 7/1/97-6/30/98; \$85,024 for PRW projects in 7/1/98-6/30/99).

United Technologies Research Center.

Unrestricted grant in "Combustion Chemistry," \$25,000, 8/1/96-12/31/96.

Naval Research Laboratory, Office of Naval Research.

"Flame Mechanism for Heptafluoropropane," \$7,333.40, 8/1/96-12/31/96.

Dow Chemical Company.

Unrestricted grant in "Fundamental Kinetics of Hydrocarbon/Chlorine Flames," \$3,000, 12/27/96.

National Environmental Technology for Waste Reduction Institute (NETI).

"Fuel-Rich Kinetics for Controlling NO_x at the Source," \$50,000, 7/1/97-6/30/98.

National Science Foundation, Course and Curriculum Development of Undergraduate Education; under subcontract from CACHE Corporation.

"WWW-Based Modules for Introduction of Molecular Simulation into the Chemical Engineering Curriculum", \$30,000 of \$332,880 for three years, 7 co-PI's; Grant #9752243, 7/1/98-6/30/02.

National Environmental Technology for Waste Reduction Institute (NETI).

"Exploiting Metallocene Catalysis," \$20,000 per year out of \$100,000 per year, 7/1/98-8/31/01 (with K. M. Ng, V. M. Rotello, M. Tsapatsis, and D. G. Vlachos).

U.S. Department of Energy.

"Probing Flame Chemistry with MBMS, Theory, and Modeling" (Grant No. DE-FG02-91ER14192, renewal) \$315,600, 7/1/98-3/31/02.

National Science Foundation.

"Research Equipment Grant: High-Performance Computing and Graphics Equipment for Research in Applied Molecular and Materials Modeling," \$86,688 (Grant 9904242 with PI P.A. Monson, Co-PI's D.G. Vlachos and P.R. Westmoreland; includes \$32,230 in U-Mass matching funds), 6/1/99-5/30/00.

U.S. Federal Aviation Administration.

"Fire-Safe Polymers and Polymer Composites," \$904,035 (P.I.: Richard Farris; Co-P.I.'s: Simon Kantor, Alan Lesser, Phillip R. Westmoreland). 7/1/99-6/30/02.

U.S. Department of Energy.

"Supplement to 'Probing Flame Chemistry with MBMS, Theory, and Modeling' (Supplemental Capital Equipment: Mass Spectrometer)" (Grant No. DE-FG02-91ER14192), \$60,000, 9/15/99-6/15/00.

Molecular Simulations, Inc.

"Molecular Dynamics Simulations of the Thermal Degradation of Bisphenol C Polycarbonate and Other Important Polymers," S.I. Stoliarov, P.R. Westmoreland, and M.R. Nyden (NIST), co-P.I.'s. \$20,000 of software, December 1, 2000.

National Environmental Technology for Waste Reduction Institute (NETI).

"Developing Mechanistic Predictions of PAH Pollutant Formation," \$20,000, 4/1/01-8/31/01.

United Technologies Research Center.

"Flame Chamber and Molecular-Beam Mass Spectrometer," \$125,000, 8/1/01.

National Environmental Technology Institute (NETI).

"Developing Mechanistic Predictions of PAH Pollutant Formation," \$50,000, 9/1/01-8/31/02.

"Mechanistic Predictions and New Monitoring Methods for PAH Pollutants," \$45,000, 9/1/02-3/31/04.

Hewlett-Packard Company.

"Connecting Molecular Models and Process Systems: Challenge Problems for Chemical and Materials Education" (PI: M.F. Malone; Co-PI's: M. A. Henson, R. S. Huss, D. Maroudas, P. R. Westmoreland) \$144,741, 9/1/03.

U.S. Department of Energy.

"Probing Flame Chemistry with MBMS, Theory, and Modeling" (Grant No. DE-FG02-91ER14192, renewal) \$220,000, 4/1/02-3/31/04.

National Science Foundation.

"A Multiprocessor Computing System for Nanoscale Science and Engineering Research in Chemical Engineering," \$55,600 (Grant 0417770 with PI P.A. Monson, Co-PI's P.R. Westmoreland and D. Maroudas; plus UMass matching funds), 4/1/04-3/31/05.

U.S. Federal Aviation Administration.

"Fire-Safe Polymers and Polymer Composites," \$846,823 (P.I. and four Co-P.I.'s). 7/1/02-6/30/06. \$275,015 Y1, \$282,758 Y2, \$289,050 Y3. No-cost extension to 2007.

Center for UMass-Industry Research on Polymers.

"Cluster F: Fire-Safe Polymers and Polymer Composites," Approximately \$250,000 per year (P.I. and four to five Co-P.I.'s). 7/1/1994-8/26/2009.

U.S. Department of Energy (T.J. Mountziaris, fiduciary co-PI during 7/2006-8/2009).

"Probing Flame Chemistry with MBMS, Theory, and Modeling" (Grant No. DE-FG02-91ER14192, renewal) \$450,000, 9/1/04-11/30/09.

Teragrid (NSF-sponsored).

"Development of Smoothly Transitioning Reactive Forcefields Based on Valence-Bond Descriptions." 28,350 service units on Copper and Cobalt supercomputers (National Center for Supercomputing Applications), TG-CTS060029N, 5/1/2006-7/30/2008.

Spectral Energies LLC.

"Establishing a Practical and Accurate Combustion Mechanism for JP-10," \$29,974.55 subcontract under \$69,921.38 Navy STTR Phase 1 contract, 8/17/2009-3/31/2010.

Teragrid (NSF-sponsored).

"Development of Reactive Molecular Dynamics and Reaction Thermochemistry." 41,500 service units on Ember and Cobalt supercomputers (National Center for Supercomputing Applications), TG-CTS090056 (XSEDE) and TG-CHE100121 (Teragrid), 11/26/2009-11/25/2010.

Internet2.

"NCSU CI Days: The Excitement and Future of CI" (Grant No. CBT-88-05703), \$18,000, 4/1/2010 - 5/1/2011.

XSEDE (NSF-sponsored).

"Reaction Kinetics and Thermochemistry for Lignocellulosic Biofuel Production." 235,000 service units on Pople and Blacklight supercomputers (Pittsburgh Supercomputing Center), 9/30/2010-3/30/2013.

National Center for Supercomputing Applications (NCSA).

"NCSU CI Days: The Excitement and Future of CI" (Grant No. TG-CTS090056), units (cpu-hours) on the Cobalt supercomputer, 4/1/2010 - 5/1/2011.

Catalysis Center for Energy Innovation, University of Delaware.

"Kinetics and Thermochemistry of Biomass Pyrolysis," Subcontract from US DOE EFRC, \$83,589, 8/1/2010-12/31/2011.

U.S. Department of Energy, National Renewable Energy Laboratory, through subcontract from RTI International.

"Kinetics of Biomass Pyrolysis and Hydropyrolysis," \$172,713, 2/1/2012-8/31/2013.

U.S. Department of Defense, Army Research Office.

"MURI: Spray and Combustion of Gelled Hypergolic Propellants," \$226,622 portion of \$3,750,000 total, 6/1/08-5/31/14. Subcontract from Purdue University.

U.S. National Science Foundation.

"Combustion Cyberinfrastructure Action-Plan Workshop," \$7,824. 3/1/2012 to 8/31/2014.

U.S. Department of Defense, Air Force Office of Scientific Research.

"Stationary Mixed Metal-Oxide Acid Catalysts for Endothermic Fuel Decomposition and Enhanced Ignition/Flame Holding Characteristics," \$300,000 portion of overall grant, 9/30/12-11/29/2015. Subcontract from University of Virginia.

E. I. du Pont de Nemours and Company / Chemours.

"Building a refrigerant combustion model," \$73,251. 8/1/2014 to 6/30/2015.

XSEDE: Extreme Science and Engineering Discovery Environment (NSF-sponsored).

"Reaction Kinetics and Thermochemistry for Lignocellulosic Biofuel Production," 125,200 service units on Ember (SGI Altix, NCSA). Award period: 7/1/2014-6/30/2016.

XSEDE: Extreme Science and Engineering Discovery Environment (NSF-sponsored).

"Reaction Kinetics and Thermochemistry for Lignocellulosic Biofuel Production," Award TG-CHE100121, 92,000 service units on comet (SDSC). Award period: 7/1/2016-12/31/2017.

U.S. National Science Foundation.

Supplement to NSF Award 1340609, "CC-NIE Networking Infrastructure: Data Intensive e-Science and SDN at NCSU" (PRIME Database Support), \$30,609. 8/1/2014 to 7/31/2016.

Eastman Chemical Company.

"Detection of Transient Intermediates at High Temperatures," \$201,525. 11/1/2012 to 8/31/2016.

"EMN-16-F-E-XX: Supplement Project Plan," \$30,000, 12/01/2016 - 08/31/2017.

U.S. Department of Energy.

"Clean Energy Smart Manufacturing Innovation Institute," PI: James Davis, \$70 million plus \$70 matching funds, 1/1/2017-12/32/2021. PRW was Director of the Southeastern Regional Manufacturing Center (\$639,147 in 1/1/2017-6/30/2017; estimate \$6 million in each year 7/1/2017-6/30/2018, 7/1/2018-6/30/2019, 7/1/2019-6/30/2020; estimate \$9 million in 7/1/2020-12/31/2021).

U.S. National Science Foundation.

"UNS: Establishing Elementary Mechanisms of Biomass and Hemicellulose Torrefaction," Award 1512401, \$309,550. 7/01/2015 to 6/30/2018.

Eastman Chemical Company.

"EMN-18-S-S-01 Esterification Mechanisms," \$123,458. 7/1/2018 to 12/30/2019.

Eastman Chemical Company.

"EMN-18-F-S-02 Fluid Degradation," \$183,609. 1/1/2019 to 12/30/2020.

U.S. National Science Foundation.

"UNS: Collaborative Research: Multiple-Scale Investigation of Chemical Looping with Oxygen Carrier Uncoupling," Award 1510900, \$309,172. 5/1/2015-4/30/2020. Co-PI with Fanxing Li (NCSU), collaborative proposal with Hanjiang Tian of West Virginia University.

XSEDE: Extreme Science and Engineering Discovery Environment (NSF-sponsored).

"Reaction Kinetics and Thermochemistry for Sugar and Polysaccharide Decomposition," Award TG-CHE100121, 92,000 service units on comet (San Diego Supercomputer Center). 7/1/2018-9/31/2019.

RAPID Process Intensification Institute (AIChE).

"Modular Conversion of Stranded Ethane to Liquid Fuels," \$1,368,292 of \$4,104,909 total. Co-PI with Fanxing Li, Henry Lamb, Tiegang Fang. Award period: 01/01/2018 - 6/30/2022.

U.S. Department of Energy, Savannah River National Laboratory.

"EM-Heated Catalytic Reaction Engineering for Polymer Deconstruction," \$85,000. Subcontract Task Order Agreement 0000508748. Award period: 01/08/2021 - 1/7/2022.

U.S. Environmental Protection Agency.

"Predictive Chemical Models for PFAS Pyrolysis and Incineration," \$237,612, two years. Award period: 5/1/2022 - 8/31/2024.

III. EDUCATIONAL ACTIVITIES

III.A. Students supervised

III.A.1. Ph.D. Students

Scott D. Thomas	"Molecular-Beam Mass Spectrometry and Mechanistic Modeling of Lean and Rich Propene Flames" (September 1992).
Roberto A. Pugliese, Jr.	"Reaction Kinetics of Plasma-Enhanced Chemical Vapor Deposition" (January 1993).
Wen Shi	"Fundamental Chemistry of Steam Cracking of Propane" (September 1994).
Jeffrey W. Peterson	"State-to-State Energy Transfer in Chemically Activated Reactions" (1991-97; did not complete degree).
Anuj Bhargava	"A Molecular-Beam Mass Spectrometry Study and Modeling of Ethylene Flames" (September 1997).
Pierre-Andre Bui-Bang-Hien	"Modeling Reactive Flows near Reactive Surfaces: Catalytic Oxidation and PECVD" (May 1998).
I. Bradford Graff	"New Diagnostic Techniques for Plasma-Enhanced Chemical Vapor Deposition of Amorphous Hydrocarbon Films" (May 1998).
Karin Rotem	"Computational Quantum Chemistry Applied to NO _x Chemistry and New Fire-Resistant Polymers" (September 1998).
George E. Oulundsen, III	"Measurements and Kinetics for Hydrocarbon-Chlorine and Allene-Doped Ethylene Flames" (August 1999).
Huiqing Zhang	"Fire-Safe Polymers and Polymer Composites" (September 2003); jointly supervised with Prof. Richard J. Farris, PSE.

Thierry Carrière	"Combustion Modeling of Ethylene/Oxygen and Allene/Oxygen Mixtures: Chemical Oxidation Mechanisms and Numerical Solution of the Non-Adiabatic Flame Equations" (April 2004).
Matthew E. Law	"Molecular-Beam Mass Spectrometry of Ethylene and Cyclohexane Flames" (August 2005).
Aurélie Schoemann	"Flammability and Pyrolysis Chemistry of Standard and Novel Fire-Safe Polymers." Jointly supervised with Prof. Richard J. Farris, PSE (Oct. 2005).
Sonia V. Tulyani	"BEBOP, A New Reactive Potential using Bond-Energy/Bond-Order Relationships," Jointly supervised with Prof. George A. Petersson, Chemistry, Wesleyan University (Sept. 2008).
Kenneth D. Smith	"Developing Reactive Molecular Dynamics for Understanding Polymer Chemical Kinetics" (March 2009).
Wenjun Li	"Initial Aromatics Growth in Different Hydrocarbon Flames" (Sept. 2011).
Nicole J. Labbe	"Determining Detailed Reaction Kinetics for Nitrogen- and Oxygen-Containing Fuels" (Dec. 2012).
Vikram Seshadri	"Pyrolysis and Combustion Kinetics of Biomass-Related Compounds" (Sept. 2014).
Patrick Fahey	"Alcohol and Saccharide Model-Compound Pyrolysis Experiments to Improve Understanding of Cellulose Pyrolysis" (2015).
Craig D. Needham	"Crafting Detailed Kinetic Mechanisms for Gas- and Condensed-Phase Systems using Computational Quantum Chemistry" (2016).
Scott D. Crymble	"Hydrocarbon Pyrolysis" (2012-2015; did not complete degree).
Charles J. McGill	"Computed Elementary Mechanisms of Homogeneous Catalysis by Saccharide-Derived Hydroxyls, Organophosphorus, and Organotin" (2019).
Sara Jo Taylor	"Kinetics of Homogeneous Catalysis by Triethyl Phosphate" (2012-2020; did not finish).
Arnab Bose	"Polysaccharide and Heat-Transfer-Fluid Pyrolysis Mechanisms Developed Using Data, Theory, and Machine Learning" (2021).
Yuan Tian	"Redox Properties of Mixed Metal Oxides for Chemical Looping Combustion and Beyond," co-advised with Dr. Fanxing Li (2022).
C. Claire Murphy	Elementary reaction mechanisms of polymer pyrolysis and PFAS incineration, 1/2021 to 8/2024; changed advisor and project.
Tim J. Mallo	Elementary reaction mechanisms of polymer pyrolysis, 12/2022 to present.
Adam Dumas	Elementary reaction mechanisms of polymer pyrolysis, 10/2023 to present.
Mahshad Manouchehri	Elementary reaction mechanisms of Novichok destruction, 1/2025 to present.

III.A.2. M.S. Students (with thesis)

Francine Communal (Fayolle)	"Plasma Measurements and Gas-Phase Kinetics in Silicon Deposition by PECVD" (September 1990).
Melissa G. Michaud (Wadkinson)	"Modeling and Measurement of Pollutants in Flames" (September 1992).
Daniel J. Hennessey	"Applying Reaction Theory in Modeling Ethene Flames" (September 1994).
Taline Inguilizian	"Correlating Polymer Flammability Using Measured Pyrolysis Kinetics" (January 1999).
Rishi R. Gupta	"Reaction Engineering Aspects of Homogeneous Catalysis and of Combustion" (July 2003).
Mikael Vienneau	"Analyzing Levels of Polycyclic Aromatic Hydrocarbons Produced in Fuel-Rich Ethylene Flames" (April 2004).
Aude Morel (Ramat)	"Molecular-Beam Mass Spectrometer Measurements and Modeling of Propene and Related Flames" (April 2005).
Saugata Gon	"Molecular-Beam Mass-Spectrometric Analyses of Hydrocarbon Flames" (October 2007).
Michael J. Gerber	"Investigation of Oxygen Exchange and Methane Combustion Kinetics for CaMnO ₃ -based Oxygen Carriers" (July 2017, co-advised with Fanxing Li; did not complete degree).

Amrutha Raghu	"Reaction Paths for Hemicellulose Pyrolysis Using Reactive Molecular Dynamics" (May 2019).
Ankush Jain	"Comparing the Pyrolyses of D-Xylose, D-Arabinose, and L-Fucose" (Dec 2020).

III.A.3. Non-thesis M.S. students.

Lu Liu	"Parallel Reactive Molecular Dynamics" (Fall 2009-Fall 2010).
Shane DiDona	"Parallel Reactive Molecular Dynamics" (Fall 2011).
Vernon Mascarenhas	"Flammability Limits from Predicted Flame Speeds" (December 2019).
Gayathri Janarthanam	"LAMMPS/ReaxFF for xylose" (August 2018-December 2019, withdrew).
Christopher Montevecchi	"Chemical looping kinetics using MBMS analysis" (1/2021-December 2021).
Madison V. Demel	"Dynamic modeling of reactive and thermal processes in chemical looping" (1/2020 to December 2021).

III.A.4. Post-doctoral associates and supervised research staff

Dr. Sreedhara Rao V.	"Computational Chemistry for NO _x Kinetics" (1996-98).
Dr. Stanislav I. Stoliarov	"Computational Chemistry for Polymer Decomposition" (2000-2002).
Dr. Hari Singh	"Computational Chemistry for Polymer Decomposition" (2002-2003).
Dr. Andrey Pereversev	"Reactive Molecular Dynamics" (2008-2009).
Dr. Young Seok Kim	"Combustion Chemistry from MBMS and Modeling" (2009-2010).
Dr. Xueliang Yang	Research Assistant Professor (2010-2012).
Dr. Xinglian Geng	Senior Research Associate (2013).
Dr. Charles J. McGill	Consultant on Eastman project "Condensation polymerization transition states" (2019).
Ms. Amrutha Raghu	"Eastman Chemical: Condensation polymerization transition states" (June-December 2019)
Dr. Haiying Wang	"Catalytic pyrolysis of lignin" (July 2019-Sept. 2020, co-advised with Dr. Li).

III.A.5. Visiting researchers.

Xin Tian, Wuhan Univ.	"MBMS Studies of Chemical Looping" (2017-2018).
Yuki Furutani, Kyushu Univ.	"Biomass pyrolysis: Lignin" (Aug-Sept 2017).
Peng Wang, Tianjin Univ.	"Biomass pyrolysis" (Jan-May 2018).

III.A.6. Thesis committees (109)

1. Daniel F. Seiter, "Oxygen Enrichment via Facilitated Transport," V. Haensel, M.S. Thesis Supervisor (Completed Spring 1989).
2. Robert E. Engle, "The Incentive for Dynamic Control in Conceptual Process Design," J. M. Douglas, Ph.D. Dissertation Supervisor (Not completed; statute of limitations expired 1990).
3. Carl V. Wikstrom, "Molecular-Beam Mass Spectrometer Sampling from an Atmospheric-Pressure Jet-Stirred Combustor," J. B. Howard and J. P. Longwell, Ph.D. Dissertation Supervisors (Massachusetts Institute of Technology, Department of Chemical Engineering; Completed January 1990).
4. Cory K. Finn, "Adaptive Process Control: Modelling, Estimation, and Control of Constrained Multivariable Systems," B. E. Ydstie, Ph.D. Dissertation Supervisor (Completed Summer 1990).
5. John E. Finn, "Molecular Theory of Adsorption Equilibria, Wetting Transitions, Multilayer Adsorption, and Adsorption from Liquid Mixtures," P. A. Monson, Ph.D. Dissertation Supervisor (Completed Summer 1990).
6. Sanjay Joshi, "Identification and Evaluation of Control Structures at the Conceptual Design Stage for Improved Control," J. M. Douglas, Ph.D. Dissertation Supervisor (Completed Spring 1991).
7. Madjid A. Kemache, "Design and Analysis of Crystallization Processes," K. M. Ng, M.S. Thesis Supervisor (Completed Spring 1991).
8. Henry A. Kusch, "Continuous Chaotic Mixing of Viscous Liquids," J. M. Ottino, Ph.D. Dissertation Supervisor (Completed Spring 1991).
9. Fernando J. Muzzio, "Nonlinearity, Chaos, and Self-Similarity: Effects of Mixing, Aggregation, Reaction, and Breakup on Structure Formation," J. M. Ottino, Ph.D. Dissertation Supervisor (Completed Spring 1991).

10. Stephen S. Jones, "Synthesis of Monometallic and Heterobimetallic Functionally Substituted Cyclopentadienyl Transition Metal Compounds," M. D. Rausch, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; withdrew, Fall 1991).
11. Vincent Gerbaud, "Study of the Electronic Structure of the Non-Bridging Oxygen Hole Center Defect in Amorphous Silica Using a Density Functional Method," M. R. Cook, M.S. Thesis Supervisor (Completed Spring 1992).
12. Erich S. Hegenberger, "Magnetic Separation of Oxygen from Air," V. Haensel, Ph.D. Dissertation Supervisor (Terminated Spring 1992).
13. David J. Mazzaresse, "Mechanistic Analysis of III-IV Semiconductor Growth via Metal Organic Chemical Vapor Deposition," W. C. Conner, Ph.D. Dissertation Supervisor (Completed Spring 1993).
14. George J. Buzad, "Design of Kinetically Controlled Reactive Distillation Columns," M. F. Doherty, Ph.D. Dissertation Supervisor (Completed Summer 1994).
15. David H. Sullivan, "Solid-State Catalyst Transformations during Oxidation Reactions over Vanadium Oxide," M. P. Harold, Ph.D. Dissertation Supervisor (Completed Summer 1994).
16. Susan R. Dye, "Separation by Crystallization," K. M. Ng, Ph.D. Dissertation Supervisor (Completed Fall 1994).
17. Richard A. Shandross, "Destruction and Growth Reactions of Important Soot Precursors in Flames," J. B. Howard and J. P. Longwell, Ph.D. Dissertation Supervisors (Massachusetts Institute of Technology, Department of Chemical Engineering; completed September 1995).
18. Priscilla J. Hill, "A Framework for Computer-Aided Design of Solids Processes," K. M. Ng, Ph.D. Dissertation Supervisor (Completed Fall 1995).
19. Alberto Nisoli, "Attainable Regions for Reaction with Separation," M. F. Doherty and M. F. Malone, M.S. Thesis Supervisors (Completed Summer 1996).
20. Katrina S. Werpetski (Gaetano), "A grid-free density-functional method and its application to inversion, torsion, and reaction potential energy surfaces," M. R. Cook, Ph.D. Dissertation Supervisor (Completed Summer 1996).
21. Boijayanta K. Bezborua, "Kinetics and Design of Ozonation Contactors," D. A. Reckhow, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Civil Engineering; Completed Spring 1997).
22. Paul Becotte-Haigh, "Overcoming Matrix Effects in Analytical Chemistry," J. Tyson, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed Spring 1997).
23. Mark C. Lovallo, "Preparation and Characterization of Zeolite Thin Films and Membranes," Michael Tsapatsis, Ph.D. Dissertation Supervisor (Completed Fall 1997).
24. Matthew J. Okasinski, "Design Methods for Kinetically Controlled, Staged Reactive Distillation Columns," M. F. Doherty, Ph.D. Dissertation Supervisor (Completed July 1998).
25. Robert G. Hynes, "The High-Temperature Oxidation and Pyrolysis Kinetics of a Hydrofluorocarbon," J. Mackie and A. Masri, Ph.D. Dissertation Supervisors (University of Sydney, School of Chemistry and Department of Mechanical and Mechatronic Engineering; Completed January 1999).
26. Jennifer Stewart, "Synthesis and Characterization of Flame-Retardant, Low-Heat-Release Polymers," R.J. Farris and B. M. Novak, Ph.D. Dissertation Supervisors (University of Massachusetts, Department of Polymer Science and Engineering; Completed Spring 1999).
27. Perry L. Mar, "Theoretical Analysis of Reaction Channels and Rate Constants in Combustion Reactions," M. R. Cook, Ph.D. Dissertation Supervisor (Completed Spring 2000).
28. Young K. Park, "Homogeneous and Platinum-Catalyzed Combustion of Hydrogen and Methane: Investigation of Bifurcation Features and Its Influence on Reactor Operation," D.G. Vlachos, Ph.D. Dissertation Supervisor. (Completed Spring 2000).
29. Jon Allan Sanborn, "Part I. A carbon-13 NMR labeling study of the Wessling polymerization. Part II. Using DFT methods to probe open shell molecules: Problems and prospects"; P. Lahti, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry, Completed Spring 2000).
30. Ketan Samant, "Design of Reaction Systems: Systematic Methods Based on a Multiscale Framework," K.M. Ng, Ph.D. Dissertation Supervisor (Completed Summer 2000).
31. Christopher D. Palmer, "The Development and Application of Instrumentation for the Spectroscopic Determination of Trace Elements," J. Tyson, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry, Completed December 2000).

32. John Husband, "Photofragmentation Studies of Transition Metal Cation-Hydrocarbon Adducts," R. Metz, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry, Completed Spring 2001).
33. Burak Esat, "Design and Synthesis of Nitronyl Nitroxide and Iminoyl Nitroxide Radicals as Organic Molecular Magnetic Materials and Their Metal Chelates as Magnetic Materials," P. M. Lahti, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry, Completed Spring 2001).
34. Fernando Aguirre, "Electronic Spectroscopy of AuCH_2^+ and Intermediates Involved in the Conversion of Methane to Methanol by FeO^+ ," R. Metz, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; completed Spring 2002).
35. Sagar Gadewar, "Feasible Regions for Reactive Distillation," M.F. Doherty and M.F. Malone, Ph.D. Dissertation Supervisors (Completed Spring 2002).
36. Kieron Faherty, "The Study of Solvated Transition-Metal Clusters in the Gas Phase Using a Novel Pulsed Electrospray Time-of-Flight Mass Spectrometer," R. Metz, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed Spring 2002).
37. Adam Zerda, "Molecular and Nanoscale Reinforcement of Polymers," Alan Lesser, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Polymer Science and Engineering; Completed Summer 2002).
38. Yang Liu, "Design and Control of Solid Processes," K.M. Ng and A.Q. Zheng, M.S. thesis supervisors (Completed Summer 2002).
39. Anonymous M.S. thesis student, Kuwait University; service as M.S. thesis Reader (thesis review) July 2002.
40. Richard Maldanis; "Group IV transition metal catalysts for the polymerizations of olefins," Marvin Rausch, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed Spring 2003).
41. Paul Serwinski, "Synthesis of Open-Shell Organic Molecules for Magnetic Materials Applications and Investigations," Paul Lahti, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed June 2003).
42. Marianny Yajaira Combariza, "Exploring Ion-Molecule Reactions in a Quadrupole Ion Trap as a Tool to Obtain Coordination Structure from Transition Metal Complexes," Richard Vachet, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed Summer 2003).
43. Christopher Thompson, "Electronic Spectroscopy and Dissociation Dynamics of Cationic Transition Metal Species," R. B. Metz, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed Summer 2003).
44. Shailendra Gupta, "Structured Liquid Products: Non-Newtonian Effects in Emulsification Processes," S. R. Bhatia and M. F. Malone, M.S. Thesis Supervisors (Completed January 2004).
45. Matthew J. Frain, "Investigation of the Influence of Gas and Solid Particle Interaction on the Heat Transfer Effectiveness of a Falling-Bed Heat Exchanger, David Schmidt, Ph.D. Dissertation Supervisor (University of Massachusetts, Department of Mechanical and Industrial Engineering; Completed April 2004).
46. Amanda Chaparro, "Study of the Dissociation Dynamics of Transition Metal Complex Ions," Richard Vachet, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed June 2004).
47. Stephanie Smulligan: "Lanthanide-Based Olefin Catalyst Precursors," P. Bianconi, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; withdrew without degree, 2004).
48. Maohua Cao; "Molecular Modeling of Solid-Fluid Equilibrium of Complex Molecules," P.A. Monson, Ph.D. Dissertation Supervisor (Completed May 2005).
49. Shoujun Bian; "Nonlinear Modelling, Estimation, and Predictive Control of Cryogenic Air Separation Columns," M.A. Henson, Ph.D. Dissertation Supervisor (Completed May 2006).
50. Murat Citir, "Photodissociation spectroscopy"; R. B. Metz, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; Completed August 2007).
51. Jennifer Gagliardi LaForest, "Photofragment Spectroscopy and Photodissociation Dynamics of Solvated First-Row Transition-Metal Divalent Cations"; R. B. Metz, Ph.D. Dissertation Supervisor (University of Massachusetts Amherst, Department of Chemistry; on leave of absence since 2005).
52. Jin Yang, research on high-performance reactive molecular dynamics (supervised 2008-09; withdrew).

53. Devin Yeates, Univ. of California, Berkeley, Mechanical Engineering (two years on committee; Ph.D. 2011; Michael Y. Frenklach, advisor).
54. Ravish Malik, "Computer Simulation of Protein-like Copolymers (PLCs)" (Carol K. Hall and Jan Genzer, Ph.D. Dissertation Co-advisors; Completed 7/2011).
55. Liangliang Huang, "Removal of Toxic Gases by Intercalation and Reactive Adsorption" (proposal 11/2009, Keith Gubbins, Ph.D. advisor; Completed July 2012).
56. Yun Long, "Pressure Tensor of Adsorbate in Nanoporous Materials: Molecular Simulation Studies," (Keith Gubbins, Ph.D. advisor; Completed October 2012).
57. Benjamin Gaddy, "Predictive Calculations of Defects in Thin-Film Heterostructures," NCSU Materials Science and Engineering (Douglas Irving, Ph.D. advisor; Completed 4/2013).
58. Lauren Ridge, "Predicting the Nature of the Protein Corona Surrounding Nanoparticles Using Computer Simulation" (Carol K. Hall, Ph.D. advisor).
59. Patrick R. Keene, NCSU, Mechanical Engineering (Tarek Echehki, M.S. advisor).
60. Mohammed R. Khan, "A frequency shifting liquid metal antenna with pressure," M.S. 8/2011, NCSU Chemical and Biomolecular Engineering (Michael Dickey, Ph.D. advisor).
61. Cody Addington, "Molecular Simulation of Phase Behavior, Interfacial Phenomena, and Pressure Effects in Porous Media," NCSU, Chemical and Biomolecular Engineering (Carol Hall, Ph.D. advisor; I served until my 2015-16 sabbatical; graduated 2016).
62. Janjira Hongrapipat, University of Canterbury, Christchurch, New Zealand – external examiner (Shusheng Pang, Ph.D. Dissertation Advisor; completed 10/2014)
63. Simon T. Thompson, "Palladium-Rhenium Catalysts for Production of Chemicals and Fuels from Biomass," NCSU, Chemical and Biomolecular Engineering (H. Henry Lamb, Ph.D. advisor; completed 5/2015).
64. Ezinne C. Achinivu, "Isolation and Recovery of Lignin from Lignocellulosic Biomass Using Recyclable Protic Ionic Liquids (PILs) for a Cost-Effective Biomass Processing Technique," NCSU, Chemical and Biomolecular Engineering (Wesley Henderson, Ph.D. advisor; Completed 5/2014).
65. Janjira Hongrapipat, Chemical and Process Engineering, University of Canterbury (NZ), "Removal of NH₃ and H₂S from Biomass Gasification Producer Gas" (Prof. Shusheng Pang, Ph.D. advisor; completed 11/2014).
66. Forrest G. Kidd III, "Development of a Novel Temperature Measurement Scheme Through the Two-Photon Excitation of Krypton," NCSU, Mechanical and Aerospace Engineering (Prof. Venkateswaran Narayanaswamy, Ph.D. advisor; completed 5/2015).
67. Jeffrey Miles, "ODT-Based Closure Model for Non-Premixed Combustion LES," NCSU, Mechanical and Aerospace Engineering (Prof. Tarek Echehki, Ph.D. advisor; completed 1/2017).
68. Opeoluwa Owoyele, "Accelerating the Simulation of Chemically Reacting Turbulent Flows via Machine Learning Techniques," NCSU Mechanical and Aerospace Engineering (Prof. Tarek Echehki, Ph.D. advisor, completed 12/2017).
69. Matthew D.S. Parker, "Microfluidic Synthesis of Monodisperse Yolk-Shell Titania Microspheres as Photocatalysts for Dry Reforming of Methane" (Prof. Milad Abolhasani, M.S. advisor, March 2019).
70. Yunfei Gao, "Ethylene Production with Active Lattice Oxygen under a Cyclic Redox Scheme" (Prof. Fanxing Li, Ph.D. advisor, completed 6/2019).
71. Rishikesh N. Ranade, "Development of Machine Learning Methods for Turbulence Combustion Closure and Chemistry Acceleration," NCSU, Mechanical and Aerospace Engineering (Prof. Tarek Echehki, Ph.D. advisor; completed August 2019).
72. Aravind Ramachandran, "An Experimental Study of Flame Stabilization Mechanisms in Turbulent Non-premixed Jet Flames Under Autoignitive Conditions," NCSU, Mechanical and Aerospace Engineering (Profs. Venkateswaran Narayanaswamy and Kevin M. Lyons, Ph.D. co-advisors; completed October 2019).
73. Vasudev P. Haribal. "Light Alkane Valorization using a Redox Approach" (Prof. Fanxing Li, Ph.D. advisor; completed Fall 2019).
74. Kevin Ley, "Parametric Study on the Laser Forced Ignition of Laminar and Turbulent Round Jets in Non-Ideal Environments," NCSU, Mechanical and Aerospace Engineering (Prof. Venkateswaran Narayanaswamy, Ph.D. advisor; completed March 2020).
75. Ronald J. Richards, "Teaching Hip-hop in the 'Burbs: Using Self-Study Teacher Research to Reveal a Secondary English Language Arts Teacher's Role Implementing Hip-hop Pedagogy in the Classroom"

- (NCSU, College of Education - Curriculum & Instruction, Prof. Angela Wiseman, D.Ed. advisor; completed May 2020).
76. Ryan B. Dudek, "Redox Catalysts for Selective Hydrogen Combustion" (Prof. Fanxing Li, Ph.D. Dissertation advisor; completed 10/2020).
 77. Zeynep Serinyel (Univ. Orléans), Habilitation, 2021.
 78. Alajia Renay Thornton, "Screening Different Perovskite-based Phase-Transition Sorbents for Sorption-Enhanced Steam Reforming of Glycerol" (Prof. Fanxing Li, M.S. advisor; completed 5/2022).
 79. Joseph McCaig, "Assessing the Active Sites in Ni/aluminosilicate Catalysts for Heterogeneous Ethylene Oligomerization." (Prof. H. Henry Lamb, Ph.D. advisor; completed 5/2022).
 80. Emily Krzystowczyk, "Optimization of Oxygen Sorbents for Thermochemical Air Separation" (Prof. Fanxing Li, Ph.D. advisor; completed 6/2022).
 81. Daniel Jackson (Prof. Fanxing Li, Ph.D. advisor; Entered Fall 2018; withdrew 5/2020).
 82. Bradley A. Davis, "Synthesis and Design of Polymer Network-Supported Catalysts for Continuous Flow Organic Synthesis" (Profs Jan Genzer and Milad Abolhasani, Ph.D. advisors; completed 6/2023).
 83. Junchen Liu, "Intensified Chemical Production via Chemical Looping Oxidative Dehydrogenation" (Prof. Fanxing Li, Ph.D. advisor; completed 8/2023).
 84. Nathan Weber (as his External Examiner), "Experimental and Theoretical Investigations of the Thermal Decomposition of Per- and Polyfluoroalkyl Substances (PFAS)," University of Newcastle, Department of Chemical Engineering (Eric Kennedy, Ph.D. advisor; March 2024).
 85. Abinash Sahoo, "Dynamics of Non-premixed Conventional and MILD Jet Flames under Autoignitive Conditions," NCSU, Mechanical and Aerospace Engineering (Profs. Venkateswaran Narayanaswamy and Kevin M. Lyons, co-advisors; entered Fall 2018, completed 9/2024).
 86. Leo Grant Brody, "Perovskite-based Phase Transition Sorbents for CO₂ Sorption-Enhanced Oxidative Steam Reforming" (Prof. Fanxing Li, advisor; Ph.D. completed 10/23/2024).
 87. Sherafghan Iftikhar, "Thermochemical CO₂ Splitting via Redox Metal Oxides: A Pathway Towards Sustainable Chemical Production" (Prof. Fanxing Li, advisor; Entered Fall 2019; completed 5/2024).
 88. Kaushik Nonavinakere Vinod, "Flash Boiling Behavior and Spray Dynamics of Liquid Ammonia as a Future Fuel: An Experimental Investigation," NCSU, Mechanical and Aerospace Engineering (Prof. Tiegang Fang, advisor; entered Fall 2021, completed 12/13/2024).
 89. Ryan DeBoskey, "Investigation of Solid Fuel Ramjet Combustion Dynamics through Integrated Experimental and Numerical Approach," NCSU, Mechanical and Aerospace Engineering (Prof. Venkateswaran Narayanaswamy, advisor; entered Fall 2022).
 90. Kevin Mangala Gitushi, "Data-based Machine Learning Models for Reduction and Acceleration of Turbulent Combustion Closure and Combustion Chemistry," NCSU, Mechanical and Aerospace Engineering (Prof. Tarek Echekki, advisor; Ph.D. completed 11/22/2024).
 91. Meghna Das Chaudhury, "Experimental and Numerical Study of Methane-Piloted, Lean, Premixed Ammonia/Methane/Air Flames in a Swirl-Stabilized Gas Turbine Can Combustor," NCSU, Mechanical and Aerospace Engineering (Prof. Srinath Ekkad, advisor; entered Spring 2021, completed 12/24/2024).
 92. Kyle J. Vogt-Lowell (Prof. Fanxing Li, advisor; Entered Fall 2019)
 93. Kevser Hilal Bektas, Chemical looping (Prof. Fanxing Li, advisor; entered Fall 2021).
 94. Mahe Rukh, Chemical looping (Prof. Fanxing Li, advisor; entered Fall 2021).
 95. Nora Khalil, "Reaction mechanism generation for fluorocarbon kinetics," Northeastern University, Chemical Engineering (Prof. Richard West, advisor; entered Fall 2022).
 96. Matthew Schram, High-speed aerodynamics and scramjet inlets. NCSU, Mechanical and Aerospace Engineering (Prof. Venkat Narayanaswamy, advisor; entered Fall 2022).
 97. Dennis Chacko (Prof. Fanxing Li, advisor; entered Fall 2019).
 98. Aaron Frye (Prof. Fanxing Li, advisor; entered Fall 2021).
 99. Sam Portillo (Prof. Fanxing Li, advisor; entered Fall 2022).
 100. Alireza Valayati (Prof. Milad Abolhasani, advisor; entered Fall 2022).
 101. Negin Orouji (Prof. Milad Abolhasani, advisor; entered Fall 2022).
 102. Adam Phengsomphone, NCSU, Mechanical and Aerospace Engineering (Prof. Venkat Narayanaswamy, advisor; entered Fall 2022).
 103. Dakshaka Hettikankanange, NCSU, Mechanical and Aerospace Engineering (Prof. Tarek Echekki, advisor; entered Fall 2023).
 104. Syedamin Razavi, Chemical looping (Prof. Fanxing Li, advisor).
 105. Casey Gilmer, Phase-transition Perovskites (Prof. Fanxing Li, advisor; entered Fall 2023).

106. Gavin Gaynor, Delignification of miscanthus in butanol/water systems (Prof. Lucian Lucia, advisor; NCSU Forest Biomaterials; entered 2021).
107. Moritz Woelk (Prof. Wentao Wang, advisor; entered Fall 2023).
108. Mabel Barreiro Carpio (Profs. Yevgeny Brudno & Joshua Pierce, advisors; NCSU Chemistry; entered Fall 2023).
109. Nisarg Joshi (Dean Jim Pfaendtner, advisor; Transfer from U. Washington, Spring 2024)
110. William Martin (Prof. Fanxing Li, advisor).

III.A.7. Undergraduate (55) and high-school (3) independent-study students

- Aug 24-May 25 Jasmine Prabawa, Pyrolysis yields from polymers.
 Aug 24-May 25 Lydia Walston, Pyrolysis yields from polymers."
 Jan 24-May 25 Alex Lambrecht, RMG solvation modeling of Dowtherm A decomposition; Polymer pyrolysis.
 Jan-May 24 Rachel Crouse, Pyrolysis yields from polymers.
 Aug 23-May 24 Nick Zezza, Pyrolysis yields from polymers.
 Mar-Aug 23 Vagish Bhushan Nangia, Indian Institute of Technology, Delhi, Potassium carboxylate pyrolysis by LAMMPS/ReaxFF Reactive Molecular Dynamics.
 Jan-May 23 Jackson Lods, Neural network for GC-MS calibration factors.
 Sep 22-May 23 Noah Stallcup, Analytical instrumentation for polymer pyrolysis.
 Sep 22-May 23 Mara Fischer, Analytical instrumentation for polymer pyrolysis.
 Nov 21-May 22 Thomas P. Sadej, PFAS Modeling from Computational Quantum Chemistry and Transition-State Theory Codes.
 Nov 21-Nov 22 Jonathan Falso, Set-up of HPLC Apparatus and Computer Data Acquisition.
 Aug 21-May 25 Hrishikesh Ram, Kinetics from TGA Experiments, RMG Mechanism Generator, Computational Quantum Chemistry, and Transition-State Theory Codes.
 Aug 21-May 22 Abdulaziz Swead, Chemical Looping MBMS Experiments and Cantera Modeling.
 Aug 20-May 22 Mitchell Haselow, Kinetics of Glucose Pyrolysis from LAMMPS/ReaxFF Reactive Molecular Dynamics.
 Aug 20-Dec 21 Jared Haselow, Kinetics of Xylose Pyrolysis from LAMMPS/ReaxFF Reactive Molecular Dynamics.
 Aug 20-May 21 Katrina Bach, Installation and Execution of Flame Modeling with OpenSMOKE++.
 Aug 20-Apr 21 Jaden Leatherman (North Carolina School of Science and Mathematics), Kinetics of Glucose Pyrolysis from RMG Reaction Mechanism Generator.
 Aug 20-Apr 21 Ariana Jenkins (North Carolina School of Science and Mathematics), Kinetics of Xylose Pyrolysis from RMG Reaction Mechanism Generator.
 May 20-Apr 21 Nathan Hames (Rhodes College), "F + HFO-1234yf Kinetics."
 Jun 19-May 22 Jennifer Wang, Correlation of species identities by GC Kovats Indices; GC operation.
 Aug 19-Aug 20 Nupur Jain, Correlation of mass spectra.
 Spr-Sum 19 Emily Heckard, Thermal stability of heat-transfer fluids.
 Fall 18-Spr 19 Chris Weber, Flame velocity predictions.
 Spr 18-Fall 18 Mazin Al-Omani, Analysis of PI-MBMS Flame Data.
 Sum 17-Spr 18 Katie Cao, GCxGC TOFMS analyses of biomass pyrolysis.
 Sum 15-Su 16 Haley Key, Flow-tube MBMS analyses.
 Sum -Fall 15 Brian Gentry, Flow-tube MBMS analyses.
 Sum 15 Kristen Bowman, PrIME database development.
 Sum 15 Connor Thompson, PrIME database development.
 Sum 15 Shujun Ye, PrIME database development.
 Sum 15 Celeste McFarlane (NC School of Math and Science), "Poly(acrylonitrile) pyrolysis products."
 Fall 14-Spr 15 Joseph H. Gilliam, "Pyrolysis chemistry."
 Fall 14-Spr 15 Nicola Kelfkens, "Pyrolysis chemistry."
 Spr 13 Andrew Crothers, "VASP simulations," 1 cr, ChE 498.
 Spr 13 Jason Baker, "Analysis of Activated Carbon Production for a Tire Pyrolysis Plant," Honors Capstone Design Project; ChE 451 design project with Andrew Santos, Andrew Covington, Andrew Crothers.
 Fall 12 Cristiana Lopes-Lara, "PrIME database and cyberinfrastructure development."
 Spr 12-Jan 13 Peitong Duan, "Reactive Molecular Dynamics."

Sum-Fall 12	Charles Lane, "Lignin pyrolysis."
Fall 11-Spr 12	Andrew Crothers, "PrIME database and cyberinfrastructure development."
Spr 11-Spr 12	Jordan Keith, "Computational chemistry for biofuels."
Fall 10-Spr 11	Charles Jones, "Archiving PI-MBMS Data."
Fall 02, Sum 02	Tyler Upton, "PAH Sampling."
Sum 02	Bryan Looze, "PAH Sampling."
Sum 01	Leah Underwood (Rensselaer Polytechnic Institute), "PAH Sampling."
Fall 98	Research assistant: Kerry Z. Camp, "Pyrolysis Kinetics Modeling."
Sum 98	Kerry Z. Camp, "Pyrolysis Kinetics Modeling and Measurements," Hamilton Standard Women in Engineering/Minority Engineering Summer Internship Program.
Fall 98	Timothy Milmore, "Polymer Kinetics Modeling," ChE 396 (incomplete).
Sum 95	Tal Rencus, "MathCAD Modelling of Chemically Activated Isomerizations."
Spr 94	Dorothy R. Pikula, "Data Base of Flat-Flame Profiles," 3 cr, ChE 496.
Spr 89	Carlos M. Santos, "Steam-Cracking Research"; "Methylene + O ₂ Kinetics," 1 cr, ChE 396.
Spr 89	Michael F. Simms, "Construction of Pt-Pt/13%Rh Thermocouples," 1 cr, ChE 396.
Fall 88	Carlos M. Santos, "Design of a PECVD Apparatus with AutoCAD," 1 cr, ChE 396.
Fall 88	Jalal Ghaemghami, "Implementing Codes for Flame-Concentration Predictions," not for credit.
Spr 88	Mark D. Dadmun, "Thermodynamic Data Base for Silicon-Containing Species," 1 cr, ChE 296D (Make-up of incomplete received from W.C. Conner, 1984).
Fall 87	Michael F. Simms, "Utility and Vacuum Design for Flame MBMS Experiment," 3 cr, ChE 396.
Fall 87	Kevin D. Schott, "Computer Data Acquisition for Flame MBMS Experiment," 6 cr, ChE 696A.
Fall 87	Jalal Ghaemghami, "Implementing Codes for Flame-Concentration Predictions," not for course credit.

III.A.8. Honors thesis committees

Jordan R. Keith, "Kinetic and Thermochemical Analysis of Glucose Isomerization and Radical Degeneration of Lignin with Application to Biomass Pyrolysis": Thesis supervisor (2011-12).
 Huiya Wu, "Products of Thermal Chlorination by Theory and Experiment"; Thesis Supervisor (1995-96).
 Michael J. MacDonald; K. M. Ng, Thesis Supervisor (1990-91).

III.A.9. Undergraduate academic advisor

Approximately 12-19 undergraduate students/semester Spring 1987 to Spring 2006; 8 to 30 from Fall 2010.
 Freshman advisor for summer orientation, June/July 1987-92, 1995-99, 2001-2006.

III.B. Courses taught within the University:

NC State

Spring 2025	CHE 312-001, Transport Processes II, 3 cr, 21 students.
Fall 2024	ChE 717-001 (24 students) & ChE 717-601 (11 students), Chemical Reaction Engineering, 3 cr.; 35 total.
Spring 2024	CHE 312-001, Transport Processes II, 3 cr, 43 students.
Fall 2023	ChE 717-001 (48 students) & ChE 717-601 (15 students, plus one dropped), Chemical Reaction Engineering, 3 cr.; 64 total.
Spring 2023	CHE 312-001, Transport Processes II, 3 cr, 66 students.
Fall 2022	CHE 312-001, Transport Processes II, 3 cr, 38 students.
Spring 2022	ChE 596-038, Molecular Principles of Engineering, 3 cr, 6 students (on campus). ChE 596-613, Molecular Principles of Engineering, 3 cr, 8 students (distance learning).
Fall 2021	ChE 311-001, Transport Processes I, 3 cr., 19 students.
Summer '21	ChE 717-651, Chemical Reaction Engineering, 3 cr., 8 students.
Spring 2021	ChE 312-001, Transport Processes II, 3 cr, 62 students.
Fall 2020	ChE 717-001 (18 students+6 delayed grading) & ChE 717-601 (10 students), Chemical Reaction Engineering, 3 cr.; 34 total.
Spring 2020	ChE 312-001, Transport Processes II, 3 cr, 34 students.
Fall 2019	ChE 311-001, Transport Processes I, 3 cr., 31 students.
Spring 2019	ChE 312-001, Transport Processes II, 3 cr, 45 students.
Fall 2018	ChE 596-022, Molecular Principles of Engineering, 3 cr, 7 students.

Spring 2018 ChE 312-001, Transport Processes II, 3 cr, 59 students.
 Fall 2017 ChE 311-001, Transport Processes I, 3 cr., 72 students.
 Spring 2015 ChE 312H-001, Transport Processes II Honors, 3 cr, 30 students.
 Spring 2015 ChE 395-003, Professional Development Seminar, 1 cr., 16 students.
 Fall 2014 ChE 395-001, Professional Development Seminar, 1 cr., 27 students.
 Fall 2014 ChE 395-004, Professional Development Seminar, 1 cr., 28 students.
 Spring 2014 ChE 312-001, Transport Processes II, 3 cr, 125 students.
 Spring 2013 ChE 596-022, Chemical Principles of Engineering, 2 cr, 7 students.
 Spring 2012 ChE 312, Transport Processes II, 3 cr, 114 students (Honors and Regular sections).
 Spring 2011 ChE 312, Transport Processes II, 3 cr, 108 students (Regular section).
 Spring 2010 ChE 312, Transport Processes II, 3 cr, 117 students (Honors and Regular sections).

UMass Amherst

Spring 2009 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 3 students.
 Fall 2008 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 2 students.
 Spring 2008 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 3 students.
 Fall 2007 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 4 students.
 Spring 2007 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 3 students.
 Fall 2006 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 3 students.
 Spring 2006 ChE 402, Chemical Engineering Practice II; 3 cr, 19 students.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 3 students.
 Fall 2005 ChE 556, Chemical Principles of Engineering; 3 cr, 2 students plus 1 auditing.
 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 3 students.
 Spring 2005 ChE 391A, Professional Seminar; 1 cr, 24 students.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 5 students.
 Fall 2004 ChE 621, Thermodynamics I; 3 cr, 10 students (co-taught).
 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 3 students.
 Spring 2004 ChE 391A, Professional Seminar; 1 cr, 33 students.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 4 students.
 Fall 2003 ChE 491A, Professional Seminar; 1 cr, 33 students.
 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 3 students.
 Spring 2003 ChE 338, Separations; 4 cr, 34 students.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 4 students.
 Fall 2002 ChE 621, Thermodynamics I; 3 cr, 15 students.
 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 3 students.
 Spring 2002 ChE 338, Separations; 4 cr, 37 students.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 4 students.
 Fall 2001 ChE 697A, Chemical Principles of Engineering; 3 cr, 15 students plus 3 auditing.
 ChE 791Q, Seminar: Engineering Chemistry; 2 cr, 3 students.
 Spring 2001 ChE 446, Process Control; 3 cr, 18 students.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 3 students.
 ChE 899, PhD Dissertation; 1-7 cr, 37 students [as Graduate Program Director].
 Fall 2000 ChE 625, Chemical Reactor Design; 3 cr, 11 students (plus one auditing).
 ChE 791Q, Seminar: Engineering Chemistry; 1 cr, 2 students.
 ChE 899, PhD Dissertation; 2-8 cr, 39 students [as Graduate Program Director].
 Spring 2000 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 2 students.
 Fall 1999 ChE 791Q, Seminar: Engineering Kinetics; 1 cr, 3 students.
 Spring 1999 ENGR 191, Freshman Engineering; 3 cr, 41 students.
 ChE 597A, Chemical Principles of Engineering; 3 cr, 11 students registered; 14 attending.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 2 students.
 Fall 1998 ChE 225, Chemical Engineering Fundamentals; 3 cr, 45 students.
 ChE H01, Honors section of ChE 225; 1 cr, 7 students.
 ChE 791Q, Seminar: Engineering Kinetics; 1 cr, 3 students.
 Spring 1998 ENGR 191, Freshman Engineering; 3 cr, 54 students.
 ChE 891Q, Seminar: Applied Kinetics; 1 cr, 2 students.
 Fall 1997 ChE 225, Chemical Engineering Fundamentals; 3 cr, 52 students.

- ChE H01, Honors section of ChE 225; 1 cr, 8 students (Co-taught).
ChE 791Q, Seminar: Engineering Kinetics; 1-2 cr, 3 students.
- Spring 1997 ChE 597A, Chemical Principles of Engineering; 3 cr, 7 students registered; 12 attending.
ChE 891Q, Seminar: Applied Kinetics; 1-2 cr, 4 students.
- Fall 1996 ChE 225, Chemical Engineering Fundamentals; 3 cr, 34 students (Co-taught).
ChE H01, Honors section of ChE 225; 1 cr, 8 students (Co-taught).
ChE 791Q, Seminar: Engineering Kinetics; 1-2 cr, 5 students.
- Spring 1996 ChE 402, Chemical Engineering Practice II, section 2; 3 cr, 12 students.
ChE 891Q, Seminar: Applied Kinetics; 2 cr, 5 students.
- Fall 1995 ChE 621, Thermodynamics I; 3 cr, 11 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 5 students.
- Spring 1995 ChE 402, Chemical Engineering Practice II, sections 1 and 2; 3 cr, 36 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 6 students.
- Fall 1994 ChE 621, Thermodynamics I; 3 cr, 7 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 6 students.
- Spring 1994 ChE 402, Chemical Engineering Practice II; 3 cr, 22 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 1-2 cr, 6 students.
ChE 496, Independent Study; 3 cr, 1 student.
- Fall 1993 ChE 621, Thermodynamics I; 3 cr, 10 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 5 students.
ChE 796, Independent Study; 3 cr, 1 student.
- Spring 1993 ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 5 students.
- Fall 1992 ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 4 students.
- Spring 1992 ChE 402, Chemical Engineering Practice II; 3 cr, 20 students.
ChE 796, Independent Study; 3 cr, 3 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 5 students.
- Fall 1991 ChE 625, Chemical Reactor Design; 3 cr, 19 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 3 reg; 6 attending.
- Spring 1991 ChE 597A, Chemistry of Chemical Engineering; 3 cr, 6 students registered; 11 attending.
ChE 796, Independent Study; 3 cr, 1 student.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 5 students.
- Fall 1990 ChE 625, Chemical Reactor Design; 3 cr, 17 students.
ChE 796, Independent Study; 3 cr, 2 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 3 students.
- Spring 1990 ChE 625, Chemical Reactor Design; 3 cr, 12 students.
ChE 891Q, Seminar: Microelectronics/High-Energy Kinetics; 2 cr, 4 students.
- Fall 1989 ChE 434, Mass Transfer; 3 cr, 31 students.
ChE 791Q, Seminar: High-Energy Kinetics; 3 cr, 3 students.
ChE 891Q, Seminar: Microelectronics; 2 cr, 1 student.
- Spring 1989 ChE 625, Chemical Reactor Design; 3 cr, 11 students.
ChE 691 (47 students) and ChE 791 (34 students), Departmental Seminar; 1 cr.
ChE 791Q, Seminar: High-Energy Kinetics; 3 cr, 3 students.
ChE 891Q, Seminar: Microelectronics; 2 cr, 1 student.
- Fall 1988 ChE 420, Kinetics and Reactor Design; 3 cr, 30 students.
ChE 691 (38 students) and ChE 791 (7 students), Departmental Seminar; 1 cr.
ChE 791Q, Seminar: High-Energy Kinetics; 3 cr, 2 students.
ChE 891Q, Seminar: Microelectronics; 2 cr, 1 student.
- Spring 1988 ChE 625, Chemical Reactor Design; 3 cr, 15 students.
ChE 691 (54 students) and ChE 791 (9 students), Departmental Seminar; 1 cr.
ChE 791Q, Seminar: High-Energy Kinetics; 2 cr, 2 students.
- Fall 1987 ChE 420, Kinetics and Reactor Design; 3 cr, 23 students.
ChE 691 (55 students) and ChE 791 (11 students), Departmental Seminar; 1 cr.
ChE 791Q, Seminar: High-Energy Kinetics; 2 cr, 2 students.
- Spring 1987 ChE 333, Chemical Engineering Heat Transfer; 3 cr, 21 students.
- Fall 1986 ChE 420, Kinetics and Reactor Design; 3 cr, 27 students.

III.C. Courses and course segments taught outside the University

- Workshop: "Putting chemistry in chemical engineering classes," ASEE Summer School for Chemical Engineering Faculty, July 29 – Aug. 3, 2017, Raleigh, NC.
- Networking session (Chair): "Molecular Simulations and Thermodynamics," ASEE Summer School for Chemical Engineering Faculty, July 29 – Aug. 3, 2017, Raleigh, NC.
- "Energy in a New Golden Age of Chemical Engineering" and "Applying chemical energy science: (1) Making bio-oils by pyrolysis; (2) Burning bio-oils cleanly," two 1-1/2-hr guest lectures in Senior course on Energy, ENSIC, Université de Lorraine, Nancy, France.
- "Computational Quantum Chemistry for the Classroom", ASEE Summer School for Chemical Engineering Faculty, Pullman WA, July 30, 2007; 12 participants (invited).
- "Computational Quantum Thermochemistry for Kinetics", International Conference on Properties and Phase Equilibrium for Product and Process Design, Hersonissos Greece, May 21, 2007; 45 participants (invited).
- "Fundamentals and Applications of Quantum Chemistry" (tutorial with J. Hess), San Francisco Hilton Hotel, San Francisco CA, November 15, 2003; 5 participants.
- "Applied Molecular Modeling," 2002 Summer School for Chemical Engineering Faculty, American Society for Engineering Education, Boulder CO, July 2002; 58 participants.
- "Fundamentals and Applications of Quantum Chemistry" (tutorial with M.J. Frisch, D. Gallagher), Reno Hilton Hotel, Reno NV, November 4, 2001; 125 participants.
- "Fundamentals and Applications of Molecular and Materials Modeling" (tutorial with P.T. Cummings, P.J. Ludovice, M. Neurock), Eden Roc Resort and Hotel, Miami Beach FL, November 15, 1998; 84 participants.
- "Quantum Chemistry for Engineers and Chemists in the Chemical Process Industries" (short course with D.J. Fox, M.J. Frisch, M. Neurock), Gaussian, Inc.; University of Houston, Houston TX, January 6-9, 1998, 35 participants.
- "Quantum Chemistry for Engineers and Chemists in the Chemical Process Industries" (short course with D.J. Fox, M.J. Frisch, M. Neurock), Gaussian, Inc.; National Center for Supercomputing Applications, Urbana-Champaign, IL, June 3-6, 1997, 14 participants.
- "Filtration" and "Ultrafiltration" modules, Unit Operations Laboratory (undergraduate), Virginia Polytechnic Institute, Chemical Engineering, Blacksburg VA, 1980; 18 students.
- "Combustion Chemistry" (graduate), Massachusetts Institute of Technology, Chemical Engineering, Cambridge MA, 1982; 8 students.

IV. PROFESSIONAL AND PUBLIC SERVICE

IV.A. National and International

IV.A.1. Professional organizations

American Institute of Chemical Engineers (AIChE).

Prepare AIChE Fellow and Institute Award nomination packages (14).

Research and New Technologies Committee and Reorganization and Bylaws Committee, 2025.

Officer and Board of Directors Nominating Committee, 2022-2024.

Executive Director Search Committee member, 2021-22.

“35 under 35” Awards of the AIChE Young Professionals Committee, Mentor to organizers about process and judge selection for inaugural 2017 set, 2016-17.

Chair of Core Judging Committee, 2016-17.

Steering Committee, 2019-20.

Process Intensification Task Force, 2015-2016.

Past Presidents Committee, 2014-present.

Public Affairs and Information Committee (PAIC), Member 2014, Chair-elect 2015, Chair 2016-17, Past Chair 2018-19.

Organizer and emcee of annual “Critical Public Policy Issues for Every ChemE” session at the 2015 and 2016 Annual Meetings, extended to add Town Halls in 2017 and 2018.

Chair of Communications Subcommittee, 2019-2024.

Selection Committee for Washington Internships in Science and Engineering (WISE) program, 2022, 2023; member, WISE Sustainability Task Force, 2023.

Ethics Committee, Chair, 2014-18. [Investigation and judgement on ethics complaints with respect to AIChE members.]

Academic-Industry Goal Alignment Task Force, Co-Chair, 2014-15, 2020-21.

Continuing Education Committee, Chair, 2014-2015.

AIChE President 2013 (President-Elect 2012, Past President 2014). Tasks: Strategic Plan Review Task Force, 2013-14, Finance Committee 2012-14, Public Affairs and Information Committee 2012; Board Awards Committee chair 2014, Nominating Committee chair for 2014 and 2015 (board and officer elections), Board of Directors member for Institute for Sustainability.

AIChE Foundation Board of Trustees 2013-22.

Foundation Grants Work Process Task Force, 2019.

Grants Committee, 2018-2022, Co-Chair 2022 (selection of Foundation grants by proposal review).

Liaison to the Sustainable Energy Corps and Workshop, 2021, and ASEE/AIChE Summer School for Chemical Engineering Faculty, 2021-22.

President’s Blue-Ribbon Task Force on Local Sections, 2013-14.

President’s Blue-Ribbon Committee on Government Relations, Chair, 2010-2011.

AIChE Board of Directors, 2008-2010.

Board Liaison to AIChE Admissions Committee, 2008-10.

Board Liaison to Social Impacts Operating Council, 2008-09.

Fellows Review Committee (Board of Directors committee).

Board Awards Committee (Board of Directors committee).

2008 Centennial Celebration Committee. Leader of the “Future Thoughts” project (solicited expert opinions on 25-year future of chemical engineering, composed article for Centennial issue of *Chemical Engineering Progress*).

Dankwerts Lecture Selection Committee, US representative, 2006-2012.

Executive Board of the National Program Committee (EBPC; 1999-2006).

Board Member, At-Large (1999-2002), Second Vice Chair (2003), First Vice Chair (2003-04), Chair (2005), Past Chair (2006).

Institute Lecture Committee: Member (2000), Chair (2006)

Co-author, “National Program Committee Manual,” 2005.

Co-author, “Topical Conference How-To Guide” (with Winston Ho), 2002.

Nanoscale Science and Engineering Forum (Group 22).

Formation Committee, 2003.

Board of Directors: Liaison Director, 2003-2005; ex officio member, 2006.
Computational Molecular Science and Engineering Forum (CoMSEF; Group 21).
Board of Directors and Vice Chair for Communications, 2002-2006.
Past Chair, 2001-2002.
(Founding) Chair, 2000-2001.
Formation Committee, 1999-2000.
AIChE Discussion Group on Computational Chemistry and Its Industrial Applications. Organizer, 1993-2000.
Catalysis and Reaction Engineering, Group 20 (Until 1995: Area 1b, Kinetics and Catalysis).
Division Advisory Board: Member, 1999-2002.
Materials Science and Engineering Division (Group 8).
Program Committee, Area 8e - Microelectronics and Photonics (1993-1996).

CACHE Corporation (nonprofit corporation: Computer Aids for Chemical Engineers).
Academic Trustee, 1999-present.
President, 2004-2006.
Vice-President, 2002-2004.
Secretary, 2000-2002.
Founding Co-chair, 2000: Foundations of Molecular Modeling and Simulation (FOMMS).
Molecular Modeling Task Force, member 1998-present.
Founding Co-chair, 2019: Foundations of Process Analytics and Machine learning (FOPAM); Co-Chair 2023.
By-Laws Revision Task Force, 2021.

Combustion Institute: International.

Chair, Executive Committee Officers Nomination Committee, 2023-4.
Chair, Ad hoc Committee to Assess the Combustion Institute Fellows Program, 2022.
Board of Directors: Member, 2002-08, 2008-2014. Officer Nominations Committee, 2003; Board Nominations Committee, 2005, 2018, Chair 2020; Bernard Lewis Travel Fellowship Selection Committee, 2008, Chair 2010-2012; By-Laws Revision Committee, Chair 2010-2013; Nominations Revision Comm, 2013-2014.
Silver Medal Committee, 2015.
Gold Medal Committee, 2014.
Co-Founder, member, and first Chair of the Joint Executive Committee of the U.S. Sections, 2001-2003.
Publication Committee, 1999-2002.
Program Committee:

- 40th International Symposium on Combustion, July 21-25, 2024, Milan, Italy.
- 39th International Symposium on Combustion, July 24-29, 2022, Vancouver, Canada.
- 38th International Symposium on Combustion, January 24-29, 2021, Adelaide, Australia (virtual conference).
- 37th International Symposium on Combustion, July 29-August 3, 2018, Dublin, Ireland.
- 36th International Symposium on Combustion, July 31-August 5, 2016, Seoul, Republic of Korea.
- 31st International Symposium on Combustion, August 6-11, 2006, Heidelberg Germany.
- 32nd International Symposium on Combustion, August 3-8, 2008, Montreal Canada.
- 28th International Symposium on Combustion, July 31-August 4, 2000, Edinburgh, Scotland.
- Editorial Committee member and Program Subcommittee member, 27th International Symposium on Combustion, August 2-7, 1998, Boulder CO.
- Editorial Committee member and Program Subcommittee member, 26th International Symposium on Combustion, July 28-August 2, 1996, Naples, Italy.
- Editorial Committee and Program Subcommittee, 25th International Symposium on Combustion, July 1994, Irvine CA.
- 24th International Symposium on Combustion, July 5-10, 1992, Sydney, Australia.
- 23rd International Symposium on Combustion, July 22-27, 1990, Orléans, France.

Combustion Institute: Eastern States Section.

Successful proposal to host Eastern States Section Combustion Institute biennial technical meeting in March 2026 at North Carolina State University, 2024.
Preparation and submission of proposal to host 14th US National Combustion Meeting in March 2025 at North Carolina State University, 2023.
Past Chair, 2003-2005; Chair, 2001-2003; Vice-Chair, 1999-2001.
Papers Chair, 1997-99. Organized and published Proceedings volumes for Annual Technical Meeting, including first joint meeting of the United States sessions (March 1999).
Program Chair, 1995-97. Organized program for Fall Technical Meetings, developed and maintained section World-Wide Web pages.
Nominations Committee, 1997.
Finance Committee, 1994-95.
Member-at-Large, Executive Committee, 1993-96.

Council for Chemical Research (www.ccrhq.org).
Governing Board: Member, 2005-07; Executive Committee, 2006.
Chair, Governance Committee, 2006.
Research Collaboration Action Network: Member, 2004-2009.

Sigma Xi (Scientific research honor society). Member, elected 2020.

Smart Manufacturing Leadership Coalition (www.smartmanufacturingcoalition.org).
Governing Board: Member, 2012-2019.

RAPID, the Modular Chemical Process Intensification Institute for Clean Energy Manufacturing (<https://www.aiche.org/rapid>).
Governing Board: Member, 2018-2023.
Evaluations for culminating presentations of RAPID interns (2020-present).
Advisor to 2020-21 Chem-E Cube Competition pilot activities, including solicitation of a team from N.C. State as one of the four pilot teams.
Co-Advisor to 2023 Chem-E Cube team from NC State for the spring 2023 opening pitches.

IV.A.2. Editorial activities

Co-editor (with Prof. Martha Grover of Georgia Tech) for special six-paper section in *Chemical Engineering Education* (Oct 2022) on "Teaching Data Science to Students and Teachers."

Journal of Advanced Manufacturing and Processing.
Editorial Advisory Board, 2018-2025.

Editor and sometimes author of four "ChE in Context" columns per year in *Chemical Engineering Progress*, also of ChEnected.aiche.org blog series (as AIChE PAIC Communications Committee Chair), 2017-24.

Co-editor, "Multiscale numerical simulation of biomass thermochemical conversion," special issue of *Fuel Processing Technology* (2019). <https://doi.org/10.1016/j.fuproc.2019.106294>

International Journal of Chemical Kinetics.
Editorial Advisory Board, 2000-2002 (three-year term).

Industrial and Engineering Chemistry Research.
Editorial Advisory Board, 1998-2000.

Co-editor, "Combustion and Incineration in Chemical Engineering," special issue of *Combustion Science and Technology*, Vol. 82, No. 1-6, 1992.

IV.A.3. Study panels

Co-initiator of 2019-2022 National Academies study on “Frontiers of Chemical Engineering” with Alexander Orlov (Stony Brook University), Joan Brennecke (Notre Dame / Texas / National Academies Board of Chemical Sciences and Technology vice-chair), and Teresa Fryberger (BCST Director).

- Organized 2016 AIChE-Foundation-funded lunch summit to evaluate the need and interest in such a study.
- Raised commitments for approximately \$1.2 million from agencies, companies, and other organizations.
- Study began in February 2019.
- Worked with Eric Kaler and study's support staff as liaison for international companion studies.
- Provided presentation and led discussion for the study's Education Subcommittee: "Future Needs for Chemical Engineering Education," 2021.

Panelist, “Advanced Manufacturing” (including presentation on “Smart Manufacturing and What It Means for North Carolina”), State Energy Conference, McKimmon Center, Raleigh NC, 4/17/2018.

Panelist, “AMS Panel: Smart Manufacturing: Industrial Internet of Things,” ASME International Design Engineering Technical Conference and the Computer and Information in Engineering Conference (IDETC/CIE), Charlotte NC, August 21–24, 2016, Paper CIE-31.

Presenter, "US government, Combustion Institute, and related initiatives for data collection and analytics," Chemistry of Smart Energy Carriers and Technologies, European Cooperation in Science and Technology, Action CM1404, Istituto di ricerche sulla combustione, Naples, Italy, April 5-6, 2016. [Invited]

Co-Chair, “Chemical Engineering Academia-Industry Alignment: Expectations about New Graduates,” U.S. National Science Foundation, Survey / Workshop / Report, 2014-15.

IUPAC Task Group on "Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment," Project 2000-013-1-100, 2000-2003, and extension Project 2003-024-1-100, 10/20/2003-1/31/2014.

Chair, NSF/DOE/NIST/DARPA/ONR/NIH panel on "International Comparative Study on Applying Molecular and Materials Modeling," 1999-2001.

Invited participant, "Workshop on Modeling Coal, Char, Soot, and Other Carbon-Based Materials," US Department of Energy (Fossil Energy and Basic Energy Sciences), Germantown MD, May 27-28, 1998.

"Molecular Simulation Modules," Web-based project of the CACHE Molecular Modeling Task Force. Participant/co-author, 1997-2002.

Co-chair, Panel on "Suppression Chemistry," NIST/DOD Workshop on Next-Generation Fire Suppression Agents, Gaithersburg MD, July 11-12, 1994.

Organizing Committee, "Green Chemistry of Polymers," Workshop for EPA Green Chemistry Institute and DOE Vision 2020 Roadmap, Amherst MA, June 11-12, 1998.

Organizing Committee, “Design of a Chemical System with Targeted Properties,” DOE Vision 2020 Roadmap Conference, College Park MD, March 16-17, 1998.

Organizing Committee, NSF Workshop on "Future Directions in Engineering Applications of Molecular Simulations and Computational Chemistry," November 3-4, 1997.

IV.A.4. U.S. government, academic, and industrial advisory boards

Committee of Visitors for Chemical, Bioengineering, Environmental, and Transport Division, National Science Foundation / Directorate of Engineering, May 22-23, 2025 (report July 2025).

Technical Advisory Board, “NSF Innovations in Graduate Education: A personalized learning model for graduate STEM education,” University of Pittsburgh, Nov 2023 to present.

Industrial Advisory Board, Louisiana State University, Department of Chemical Engineering, 2011-present.

- Also reviewed technical posters for Junior/Senior Design Day, Dec. 2020, April 2021, Dec. 2021, May 2022.

Committee of Visitors for Chemical, Bioengineering, Environmental, and Transport Division, National Science Foundation / Directorate of Engineering, June 2019 (report July 2019).

Internal review for National Academy of Engineering. 2017. *Engineering Societies and Engineering Education: Proceedings of a Workshop*. [Held Jan 26-27, 2017.]

Advisory Committee, Chemical Engineering Department at Hong Kong University of Science and Technology; External Review, June 12-14, 2016.

ExxonMobil Corporate Strategic Research (CSR) Capability Reassessment, Clinton NJ, March 1-3, 2016.

External Review of the Chemical Engineering Department at the University of Utah, April 23-25, 2014.

External Review of the Chemical Engineering Department at the University of Michigan, October 26-28, 2010.

Scientific Advisory Board, High-Performance Computing Modernization Program, U.S. Department of Defense, 2001-2005, 2010-2012.

Independent Review Panel for Next-Generation Fire Prevention program, US Department of Defense and NIST, 2001-2004.

IV.A.5. Conference and session organization

10th Sino-US Joint Conference of Chemical Engineering, Beijing, China, October 15-19, 2017. Scientific Advisory Board.

Scientific Committee, First International Process Intensification Conference (IPIC1), Barcelona, Spain, October 1-5, 2017.

IConBM2016: 2nd International Conference on BIOMASS. 19-22 June 2016, Giardini Naxos-Taormina, Sicily, Italy. International Scientific Committee.

7th Sino-US Joint Conference of Chemical Engineering, Beijing, China, October 14-18, 2013. Program Committee.

2nd Middle East Process Engineering Conference (Bahrain), September 29 to October 2, 2013. Scientific Advisory Committee.

5th International Seminar on Flame Structure, Novosibirsk, Russia, July 11-14, 2005. International Advisory Committee.

NSTI Nanotechnology Conferences.

Conference Committee, 2005 Conference, Anaheim CA, May 8-12, 2005.

Conference Committee, 2004 Conference, Boston, MA, Mar. 7-11, 2004.

Conference Committee, 2003 Conference, San Francisco, CA, Feb. 23-27, 2003.

Conference Committee, 2002 International Conference on Computational Nanoscience and Nanotechnology, San Juan, PR, April 22-25, 2002.

"2nd International Conference on Multiscale Modeling: Bridging the Gap between Atomistic and Meso Scales," conference sponsored by the Knowledge Foundation, Boston MA, August 13-14, 2001. Co-Chair.

Session Chair, "Kinetics Modeling," ISCRE 13 (International Symposium on Chemical Reaction Engineering), Baltimore MD, September 26-28, 1994.

Session Chair/Co-organizer, "Gas-Phase and Surface Chemistry in Electronic Materials Processing," Symposium W, 1993 MRS Fall Meeting, Boston.

Organizer, ACS "Symposium on Combustion Chemistry," Fuel Chemistry Division, 202nd Meeting/4th Chemical Congress of North America, August 25-30, 1991, New York.

31 papers from researchers in Australia, Egypt, France, Germany, Japan, the United Kingdom, USSR, and the United States. Obtained Type SE grant from American Chemical Society Petroleum Research Fund for \$2000 to support travel expenses of invited speakers from Germany and the Soviet Union.

American Institute of Chemical Engineers (AIChE).

Catalysis and Reaction Engineering, Group 20 (Name until 1995: Area 1b, Kinetics and Catalysis):

Session Co-chair/Organizer, "In Honor of the 2024 CRE Early Career Investigator Award winner," 2025 Annual Meeting, Boston MA.

Session Co-chair/Organizer, "Destruction of PFAS," 2025 Annual Meeting, Boston MA.

Session Co-chair/Organizer, "Catalysis and Reaction Engineering for PFAS Remediation I: Incineration" (Session 110) and "Catalysis and Reaction Engineering for PFAS Remediation II: Alternatives to Incineration" (Session 186), 2024 Annual Meeting, San Diego CA.

Session Co-chair/Organizer, "In Honor of Maria Burka," 2016 Annual Meeting, San Francisco CA [co-sponsored with Group 10, CAST].

Session Co-chair/Organizer, "Combustion Reaction Engineering I and II," 2011 Annual Meeting, Minneapolis MN.

Session Chair/Organizer, "Reactor Design for Electronic Materials Processing" (Joint with 8e), 1997 Annual Meeting, Los Angeles CA.

Session Chair/Co-Organizer, "Combustion Reaction Engineering," AIChE 1993 Annual Meeting, St. Louis MO.

Session Chair/Organizer, "Combustion Reaction Engineering," AIChE 1992 Annual Meeting, Miami Beach FL.

Session Chair/Organizer, "Combustion Reaction Engineering," AIChE 1991 Annual Meeting, Los Angeles.

Session Chair/Organizer, "Combustion Reaction Engineering," AIChE 1990 Annual Meeting, Chicago IL.

Session Co-Chair, "Combustion and Reaction Engineering II. New Experimental Techniques," AIChE 1989 Annual Meeting, San Francisco CA.

Session Co-Chair, "New Experimental Techniques for High-Temperature Reacting Flows," AIChE 1987 Annual Meeting, New York NY.

Computational Molecular Science and Engineering Forum (Group 21):

Session Co-chair/Organizer, "25 Years of CoMSEF: Past, Present, and Future," 2025 Annual Meeting, Boston MA.

Session Co-organizer, "Practical Applications of Computational Chemistry and Molecular Simulation I, II, III," 2022 AIChE Annual Meeting, Phoenix AZ.

Session Co-chair/Organizer, "Practical Applications of Computational Chemistry and Molecular Simulation I & II," 2021 AIChE Annual Meeting, Boston MA.

Session Co-chair/Organizer, "Practical Applications of Computational Chemistry and Molecular Simulation and I & II," 2020 Annual Meeting, San Francisco CA (virtual).

Session Co-chair/Organizer, "Industrial Applications of Computational Chemistry and Molecular Simulation (Invited Talks)" and "Practical Applications of Molecular Modeling and Simulation I & II," 2019 Annual Meeting, Orlando FL.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I," 2018 Annual Meeting, Pittsburgh PA.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I," Session 428, 2017 Annual Meeting, Minneapolis MN.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I, II," 2016 Annual Meeting, San Francisco CA.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I, II," 2015 Annual Meeting, Salt Lake City UT.

Session Co-chair, "In Honor of Peter Cummings III," 2014 Annual Meeting, Atlanta GA.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I, II," 2014 Annual Meeting, Atlanta GA.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I, II, III," 2013 Annual Meeting, San Francisco CA.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I, II, III," 2012 Annual Meeting, Pittsburgh PA.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I, II, III," 2011 Annual Meeting, Minneapolis MN.

Session Co-chair/Organizer, "Industrial Applications of Molecular Simulation and Computational Chemistry I and II," 2010 Annual Meeting, Salt Lake City UT.

Session Co-chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I and II," 2009 Annual Meeting, Nashville TN.

Session Co-chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I and II," 2008 Annual Meeting, Philadelphia PA.

Session Co-chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I and II," 2007 Annual Meeting, Salt Lake City UT.

Session Co-chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I and II," 2006 Annual Meeting, San Francisco CA.

Session Co-chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I and II," 2005 Annual Meeting, Cincinnati OH.

Session Co-chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I, II, and III, " "Simulation of Materials Processes, " "Monte Carlo and Molecular Dynamics of Reactive Systems," 2004 Annual Meeting, Austin TX.

Session Chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I, II, and III," 2003 Annual Meeting, San Francisco CA.

Session Chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I and II," 2002 Annual Meeting, Indianapolis IN.

Co-Chair / Organizer, Topical Conference on "Applying Molecular Simulation and Computational Chemistry," 2001 Annual Meeting, Reno NV.

Session Chair/Organizer, "Molecular Modeling Development for Industrial Applications," 2000 Annual Meeting, Los Angeles CA.

Session Chair/Organizer, "Applying Molecular Simulation and Computational Chemistry I" and "Applying Molecular Simulation and Computational Chemistry II" (Area 1a and Group 20), 1999 Annual Meeting, Dallas TX.

Co-Chair / Organizer, Topical Conference on "Applying Molecular Simulation and Computational Chemistry," 1998 Annual Meeting, Miami Beach FL.

Session Chair/Organizer, "Molecular Modeling Development for Industrial Applications," 1997 Annual Meeting, Los Angeles CA.

Session Chair/Organizer, "Computational Chemistry and Its Industrial Applications," Plenary and Poster sessions, 1996 Annual Meeting, Chicago IL.

Session Chair/Organizer, "Computational Chemistry and Its Industrial Applications," Plenary and Poster sessions, 1994 Annual Meeting, San Francisco CA.

Computing and Systems Technology Division (Group 10):

Session Chair/Organizer, "Symposium Honoring CACHE Award Recipients (Invited Papers)," 2005 Annual Meeting, Cincinnati OH.

Session Chair/Organizer, "Symposium Honoring 2004 CACHE Award Recipient for Excellence in Computing in Chemical Engineering Education (Invited Papers)," 2004 Annual Meeting, Austin TX.

Materials Science and Engineering Division (Group 8):

Session Chair/Organizer, "Reactor Design for Electronic Materials Processing" (Joint with 20), 1997 Annual Meeting, Los Angeles CA.
Session Co-Chair/Organizer, "Computational Chemistry in Materials Processing," 1995 Annual Meeting, Miami Beach FL.
Session Co-Chair, "Plasma Processing: Fundamentals and Modeling," 1994 Annual Meeting, San Francisco CA.
Session Chair/Co-Organizer, "Plasma Processing I. PECVD," and "Plasma Processing II. Etching," 1993 Annual Meeting, St. Louis MO.
Session Chair/Organizer, "Gas-Phase Kinetics in Electronic Materials Processing," 1992 Annual Meeting, Miami Beach FL.
Judge of Poster Session Competition in Materials Science and Engineering Division, 1992 Annual Meeting, Miami Beach FL.

Public Affairs and Information Committee (Group 18).

Co-organizer and session co-chair. "Public Affairs and AIChE: A PAIC Town Hall," 2019 Annual Meeting, Orlando FL.
Co-organizer and session chair (stand-in). "Public Affairs and AIChE: A PAIC Town Hall," 2018 Annual Meeting, Pittsburgh PA.
Co-organizer and session chair. "Public Affairs and AIChE: A PAIC Town Hall," 2017 Annual Meeting, Minneapolis MN.
Co-organizer and session chair. "Public Affairs and Information Committee (PAIC) Briefing on Critical Public Policy Issues for Every Chemical Engineer," 2016 Annual Meeting, San Francisco CA.
Co-organizer and session chair. "Public Affairs and Information Committee (PAIC) Briefing on Critical Public Policy Issues for Every Chemical Engineer," 2016 Annual Meeting, San Francisco CA.
Co-organizer and session chair. "Public Affairs and Information Committee (PAIC) Briefing on Critical Public Policy Issues for Every Chemical Engineer," 2015 Annual Meeting, Salt Lake City UT.

Other AIChE sessions:

Co-organizer and co-chair of plenary session, Topical Conference on "Per- and Polyfluorinated Alkyl Substances (PFAS) and other Contaminants of Emerging Concern," 2025 Annual Meeting, Boston MA.
Session Co-Organizer, "Teaching Data Science to Students and Teachers," 2024 Annual Meeting, San Diego CA (CAST, Education, and CoMSEF).
Session Chair/Organizer, "NASEM Report on New Directions in Chemical Engineering and Reactions to It," 2022 AIChE Annual Meeting, Phoenix AZ.
Co-chair/Co-Organizer, "Teaching Data Science to Students and Teachers I, II, III" 2021 AIChE Annual Meeting, Boston MA.
Session Chair, "Pathways to Thermal Deconstruction," Session 501, Topical Conference of Thermal Deconstruction of Biomass, 2017 Annual Meeting, Minneapolis MN.
Session chair, "Smart Manufacturing – the Clean Energy Smart Manufacturing Innovation Institute, " Session 781, 2017 Annual Meeting, Minneapolis MN.
Session Chair/Organizer, "Public Affairs and AIChE: A PAIC Town Hall," Session 8, 2017 Annual Meeting, Minneapolis MN.
Session Chair/Organizer, "Critical Issues for Chemical Engineers," 2016 Annual Meeting, San Francisco CA.
Session Chair/Organizer, "Critical Issues for Chemical Engineers," 2015 Annual Meeting, Salt Lake City UT.
Co-organizer and session chair, Topical Conference on "Simulation Based Engineering and Science," 2010 Annual Meeting, Salt Lake City UT.
Session Chair/Organizer, "Changing the Conversation – Strategies and Opportunities for Engineers to Strengthen the STEM K-12 Pipeline," 2009 Annual Meeting, Nashville TN.
Session Chair/Organizer, "Meet-the-Candidates Poster Session," 2003 Annual Meeting, San Francisco CA.

CACHE Corporation (education nonprofit)

FOMMS conferences (Foundations of Molecular Modeling and Simulation).

Senior Advisor, FOMMS 2024, Snowbird UT, July 28-August 1, 2024.
Senior Advisor, FOMMS 2022, Lake Lawn Resort, Delavan WI, July 17-21, 2022.
Senior Advisor, FOMMS 2018, Lake Lawn Resort, Delavan WI, July 17-21, 2018.
Organizing Committee, FOMMS 2015, Resort at Mt. Hood, Welches OR, July 12-16, 2015.
Senior Advisor and Organizing Committee, FOMMS 2009, Semiahmoo Resort, Bellingham WA, July 2009.
Senior Advisor and Organizing Committee, FOMMS 2006, Semiahmoo Resort, Bellingham WA, July 2006.
Senior Advisor and Organizing Committee, FOMMS 2003, Keystone Resort, CO, July 2003.
Co-Chair, FOMMS 2000, Keystone Resort, CO, July 24-28, 2000.
FOPAM conferences (Foundations of Process/product Analytics and Machine learning).
Programming Committee, FOPAM 2026, Atlanta GA, July 26-30, 2026.
Co-Chair, FOPAM 2023, University of California Davis, Davis CA, July 30-Aug. 4, 2023.
Co-Chair, Plenary Session chair, and Rapporteur, FOPAM 2019, Marriott Stateview Hotel, Raleigh NC, Aug. 5-9, 2018.

Combustion Institute, Eastern States Section.

Session Chair, "Chemical Kinetics," 1995 Fall Technical Meeting, Worcester MA, October 15-18, 1995.
Session Chair, "Chemical Kinetics," 1990 Fall Technical Meeting, Orlando FL.
Session Chair, "Chemical Kinetics," 1989 Fall Technical Meeting, Albany NY.
Session Chair, "Pyrolysis and Oxidation Chemistry," 1986 Fall Technical Meeting, San Juan PR.

Combustion Institute (International / US National).

Session Chair: "Reaction Kinetics I," 14th US National Combustion Meeting, Westin Copley Place, Boston MA, March 16-19, 2025.
Session Chair: "Reaction Kinetics VI," 13th US National Combustion Meeting, Texas A&M University, College Station TX, March 19-22, 2023.
Session chair, "Biomass and Biofuels," 12th U.S. National Combustion Meeting, Texas A&M University, May 24-26, 2021 (virtual).
Session Chair: "Chemical Kinetics - NO_x, Ions," 31st International Symposium on Combustion, August 6-11, 2006, Heidelberg Germany.
Colloquium Co-Chair for "Reaction Kinetics," 29th International Symposium on Combustion, July 14-19, 2002, Sapporo, Japan; Session Chair.
Session chair, "Reaction Kinetics III" and "Theory and Modeling," 2nd Joint Meeting of the U.S. Sections of the Combustion Institute, March 25-28, 2001, Oakland, California.
Session Chair, "Reaction Kinetics IV," 27th International Symposium on Combustion, August 2-7, 1998, Boulder CO.
Session Chair, "NO_x and SO_x Kinetics," 26th International Symposium on Combustion, July 28-August 2, 1996, Naples, Italy.
Session Co-Chair, "Reaction Kinetics", 24th International Symposium on Combustion, July 5-10, 1992, Sydney, Australia.
Session Co-Chair, "Combustion-Generated Pollutants," Twentieth Symposium (International) on Combustion, Munich, 1986.

IV.A.6. Peer review

External reviewer, NASEM study report on *New Directions in Chemical Engineering* (2021).

Peer reviews of papers:

Advanced Materials CVD (1);
AIChE Journal (30);
ACS Omega (1);
ACS Sustainable Chemistry and Engineering (3);
ACS Symposium Series (3);
Analytical Chemistry (1);
Applied Optics (1);

BioEnergy Research (1);
Canadian Journal of Chemical Engineering (1);
Carbohydrate Research (1);
Catalysis Science and Technology (1);
Cellulose (1);
Chemical Engineering Communications (1);
Chemical Engineering Education (9);
Chemical Engineering Journal (1);
Chemistry of Materials (1);
Chemical Engineering Science (9);
Chemical Engineering Transactions (4);
Chemical Physics Letters (1);
Chemical Reviews (1);
Combustion and Flame (57);
Combustion Science and Technology (15);
Combustion Theory and Modeling (1);
Computers and Chemical Engineering (2);
Energies (1);
Energy & Fuels (23);
Environmental Progress (1);
Environmental Science (1);
Environmental Science and Technology (3);
Fuel (8);
Fuel Processing Technology (3);
I&EC Research (24);
International Journal of Chemical Kinetics (10);
International Journal of Pure and Applied Kinetics (1);
International Symposium on Chemical Kinetics (10);
International Symposium on Chemical Reaction Engineering (3);
Journal of Advanced Manufacturing and Processing (1);
Journal of Analytical and Applied Pyrolysis (1);
Journal of the American Chemical Society (6);
Journal of Chemical Physics (1);
Journal de Chimie Physique (2);
Journal of the Electrochemical Society (2);
Journal of Fluorine Chemistry (1);
Journal of Fuels Processing Technology (2);
Journal of Engineering Education (1);
Journal of Marine and Petroleum Geology (2);
Journal of Molecular Modeling (1);
Journal of Organic Chemistry (2);
Journal of Physical Chemistry A, B, C (40);
Journal of Physical Chemistry Letters (2);
Journal of Propulsion and Power (1);
Langmuir (1);
Macromolecules (2);
Maderas.ciencia y tecnología (1);
Molecular Simulation (1);
Nature Chemistry (1);
Physical Chemistry Chemical Physics (3);
Polymer (1);
Proceedings of the Materials Research Society (3);
Proceedings of the Combustion Institute (4 – Vol. 22; 7 – Vol. 23; 9 – Vol. 24; 4 – Vol. 25; 6 – Vol. 26, 5 plus plenary – Vol. 27; 5 – Vol. 28; Symposium Chair / Editor, Vol. 29; 5- Vol. 30, 1 - Vol. 34; 1; 8 - Vol. 35; 11 – Vol. 36; 6 – Vol. 37; 7 – Vol. 38; 5 - Vol. 39, 6 - Vol. 40; 4 – Vol. 41).
Proceedings of the National Academy of Science (4);

Progress in Energy and Combustion Science (1);
Progress in Reaction Kinetics and Mechanism (1);
Reviews in Chemical Engineering (1);
Science and Technology of the Built Environment (1);
SusChem (3);
SusChemEng (1);
Thermochimica Acta (1).

Peer review of proposals:

Australian Research Council (1);
Centre national de la recherche scientifique / CNRS (1);
Deutsche Forschungsgemeinschaft (1);
U.S. Department of Defense, Army Research Office (3);
U.S. Department of Defense, High-Performance Computing Challenge Awards (40);
U.S. Department of Energy (23);
U.S. DOE Innovative and Novel Computational Impact on Theory and Experiment program (7).
U.S. Environmental Protection Agency (1);
Illinois Center for Research on Sulfur in Coal (1);
Israel Science Foundation (1);
Katholieke University of Leuven, Belgium (1);
King Abdullah University of Science and Technology, KAUST (2);
McGraw-Hill (2);
National Aeronautics and Space Administration (2);
National Research Council/National Academy of Science (1);
National Science Foundation (158).
National Institute of Standards and Technology (4);
Petroleum Research Fund (6);
Renaissance Computing Institute (5);
SUNY-Buffalo (1);
University of California Energy Institute (2);
University of Massachusetts Faculty Research Grants (3);
U.S.-Israel Binational Science Foundation (1);
Wiley Publishing (1);
Villanova University (1).

Peer reviews of tenure and promotion cases (73).

IV.A.7. National Science Foundation IPA appointment

Program Officer for Combustion, Fire, and Plasma Systems program (1407) and Cyberinfrastructure activities, Chemical, Bioengineering, Environmental, and Transport Systems Division (CBET) in Engineering Directorate. July 2006 to present.

ENG Cyberinfrastructure Working Group, 2006-present.

NSF High-Performance Computing Coordinating Group, 2007-2009.

NSF Virtual Organizations Coordinating Group, 2007-2009.

Drafted and led the "Engineering Virtual Organizations" solicitation and panels, 2007.

NSF Cyber-Enabled Discovery and Innovation Working Group, 2007-2009. Drafted the "Virtual Organizations" section; organized and led panels.

Organized or co-organized and ran panels for solicitations: Nanotechnology Interdisciplinary Research Teams (NIRT), Petaflop Applications (Peta-Apps), Virtual Organizations as Sociotechnical Systems (VOSS).

Co-organizer of multi-agency-sponsored "International Assessment of Simulation-Based Engineering and Science," \$500,000 independent panel study led by Prof. Sharon Glotzer, 2007-2009, which is considered to have led to the Materials Genome Initiative.

Participated in forming the Multi-Agency Coordinating Committee for Combustion Research (MACCCR), linking NSF, NIST, DOE, NASA, AFOSR, ARO, ONR, FAA, and other funding agencies for combustion;

developed and hosted the website. Co-organizer of MACCCR-sponsored study “Transforming Combustion Research through Cyberinfrastructure,” National Academy of Science, 2011.
 Drafted and led the Engineering Directorate’s approval process for new ENG proposal requirement, “Data Management Plans,” which was largely adopted as NSF-wide policy in the GPG.

IV.A.8. Magazine articles, op-eds, and blogs.

“The Chemical Engineer in Context”, quarterly column in *Chemical Engineering Progress*; Editor & frequent author (2017-2025). Also <https://www.aiche.org/chenected/series/che-context>

P.R. Westmoreland, “ChE in Context: New Administration, Familiar Themes,” **121:1** (2025) 18.

<https://www.aiche.org/resources/publications/cep/2025/january/che-context-new-administration-familiar-themes>

P.R. Westmoreland, “Public Policy and AIChE,” *Chem. Eng. Prog.* **120:7** (2023) 28.

<https://www.aiche.org/resources/publications/cep/2023/july/che-context-public-policy-and-aiche>

C. Grounds, G.J. Gibson, P.R. Westmoreland, “Building ‘New Directions for Chemical Engineering’ — Together,” *Chem. Eng. Prog.* **120:4** (2023) 28.

<https://www.aiche.org/resources/publications/cep/2023/april/che-context-building-new-directions-chemical-engineering-together>

P.R. Westmoreland, “Chemical Engineers Tackle Climate Solutions,” *Chem. Eng. Prog.* **119:7** (2022) 18.

<https://www.aiche.org/resources/publications/cep/2022/july/che-context-chemical-engineers-tackle-climate-solutions>

S.T. Arm, P.R. Westmoreland, “The ChE in Context: Chemical Engineers and a Nuclear Renaissance,” *Chem. Eng. Prog.* **119:4** (2022) 20. <https://www.aiche.org/resources/publications/cep/2022/april/che-context-chemical-engineers-and-nuclear-renaissance>

P.R. Westmoreland, “The ChE in Context: Understanding the U.S. Chemical Safety Board,” *Chem. Eng. Prog.* **118:7** (2021) 42. <https://www.aiche.org/resources/publications/cep/2021/july/che-context-understanding-us-chemical-safety-board>

P.R. Westmoreland, N. M. Anid, “The ChE in Context: Context for AIChE’s Climate Change Policy,” *Chem. Eng. Prog.* **118:4** (2021) 22. <https://www.aiche.org/resources/publications/cep/2021/april/che-context-context-aiches-climate-change-policy>

P. R. Westmoreland, “The ChE in Context: Anticipating Policy Changes in Washington,” *Chem. Eng. Prog.* **118:1** (2021) 31. <https://www.aiche.org/resources/publications/cep/2021/january/che-context-anticipating-policy-changes-washington>

P.R. Westmoreland, M. E. Ternes, “The ChE in Context: AIChE Updates Its Climate Change Policy Statement,” *Chem. Eng. Prog.* **115:7** (2019) 16.

<https://www.aiche.org/resources/publications/cep/2019/july/che-context-aiche-updates-its-climate-change-policy-statement>

E. Fairman, P.R. Westmoreland, “The ChE in Context: Your Voice and Role in Public Outreach,” *Chem. Eng. Prog.* **114:4** (2018) 63. <https://www.aiche.org/resources/publications/cep/2018/april/che-context-your-voice-and-role-public-outreach>

M. E. Ternes, P. Westmoreland, “The ChE in Context: Members Will Shape AIChE’s Climate Change Policy,” *Chem. Eng. Prog.* **113:7** (2017) 16.

<https://www.aiche.org/resources/publications/cep/2017/july/che-context-members-will-shape-aiches-climate-change-policy>

P.R. Westmoreland, “The ChE in Context: PAIC, The ChE’s Voice in and about Government,” *Chem. Eng. Prog.* **113:4** (2017) 26. <https://www.aiche.org/resources/publications/cep/2017/april/che-context-paic-ches-voice-and-about-government>

“Chemical Engineering and Advanced Manufacturing,” author/editor in 7-part ChEnected blog series. <https://www.aiche.org/chenected/series/chemical-engineering-and-advanced-manufacturing>

P.R. Westmoreland, “Introduction to Advanced Manufacturing for Chemical Engineers,”

<https://www.aiche.org/chenected/2018/07/introduction-advanced-manufacturing-chemical-engineers>

M.E. Ternes, P.R. Westmoreland, “AIChE and the Paris Climate Agreement,” 6/2/2017

<<https://www.aiche.org/chenected/2017/06/aiche-and-paris-climate-agreement>>

P.R. Westmoreland, “The Importance of International Exchanges to Chemical Engineering,” 2/13/2017

<<https://www.aiche.org/chenected/2017/02/importance-international-exchanges-chemical-engineering>>.

P.R. Westmoreland, “The Second Phase of ChE Education,” 3-part ChEnected blog series. <https://www.aiche.org/chenected/series/second-phase-che-education>:

P.R. Westmoreland, “The Second Phase of ChE Education,” 10/23/2013

<<https://www.aiche.org/chenected/2013/10/second-phase-che-education>>.

P.R. Westmoreland, “Second Phase of Education: Mariam Al-Meer at Shell in Qatar,” 11/21/2013

<<https://www.aiche.org/chenected/2013/11/second-phase-education-mariam-al-meer-shell-qatar>

P.R. Westmoreland, “Second Phase of Education: Lane Daley at Eastman Chemical in Kingsport,”

12/4/2013 <<https://www.aiche.org/chenected/2013/12/second-phase-education-lane-daley-eastman-chemical-kingsport>>.

P.R. Westmoreland, “We Are ChE: Entering a Golden Age,” 12-part ChEnected blog series, 9/19/2012-12/20/2012, <<https://www.aiche.org/chenected/series/we-are-che-entering-golden-age>>:

1. “Entering a New Golden Age of Chemical Engineering,” 9/19/2012.

2. “ChE-style Manufacturing Moves into the Spotlight,” 9/26/2012.

3. “More ChE Manufacturing: Rebuilding the Body,” 10/3/2012.

4. “Shale Gas in the Middle of the Worldwide Energy Drama,” 10/10/2012.

5. “The New Energy Mix: Abundance and Sustainability?” 10/17/2012.

6. “Biology and ChE: Applying a Molecular Science (Part I),” 10/24/2012.

7. “Biology and ChE: Applying a Molecular Science (Part II),” 11/7/2012.

8. “ChE Computing Becomes Cyberinfrastructure,” 11/14/2012.

9. “Massively Parallel Computing and Massive Impacts for ChE” 11/29/2012.

10. “From Big Data to Smart Manufacturing,” 12/5/2012.

11. “Embracing the Breadth and the Unity of ChE,” 12/14/2012.

12. “Seizing the Future of Chemical Engineering,” 12/20/2012.

IV.B. State or region

Member, Governor’s Advisory Commission on the North Carolina Museum of Natural Sciences, 2014-2017, 2018-2021, 2021-2025 (gubernatorial appointment April 2014; re-appointed January 2018, September 2021).

External Review Panel, NC Science Museums Grant Program.

- Review of November 9, 2017.
- Review of February 27, 2018.
- Review of October 31, 2023.

Board member, North Carolina Bio-Preparedness Collaborative (NCB-Prepared), interinstitutional earmarked support for a unified all-hazards data resource for proactive surveillance to provide on-demand analytical power and significantly enhance and extend vigilance and homeland security; \$11.75M, 2010-12.

Meeting organizer/Host, 23rd Northeast Regional Meeting on Chemical Kinetics and Dynamics, Amherst MA, January 29, 2005.

Meeting organizer/Host, 14th Northeast Regional Meeting on Chemical Kinetics and Dynamics, Amherst MA, January 27, 1996.

Meeting organizer/Host, Connecticut Valley Quantum Chemistry Group: October 2002, November 2003, October 2004, November 2005.

Massachusetts Department of Environmental Protection: Technical Review Committee, “Review of scientific evidence concerning dioxin production in municipal waste incineration,” Lowell Center for Sustainable Production, University of Massachusetts/Lowell. 2002-2003.

AICHe Western Massachusetts Section: Section Chair (1988-89).

AICHe Central New England Section: Director (1989-90, 1990-92).

AICHe Knoxville-Oak Ridge Section: Public relations chair (1976), Section Secretary (1977).

IV.C. College and University

2024-2025

Chair, Search Committee for Associate Vice Chancellor for Research Computing and Data (university).
Participate in university's DEI Collaborative: network of faculty and staff working on DEI (university).

2023-2024

Participate in university's DEI Collaborative: network of faculty and staff working on DEI (university).
RLA Past Chair, advising Chair and Vice Chair. Participate in faculty open letter to the Chancellor and in planning after his response (university).
Review of COI Management Plan for Saad Khan and Tahira Pirzada (university).

2022-2023

NCSU Research Leadership Academy.

- 2022-23 Chair.
- Planning of University Research Symposium and other RLA activities for 2022 and 2023, including:
 - Co-organizer and moderator with Paula Sztjan, RLA Lunch and Learn event: "External Awards," NCSU Research Leadership Academy, 11/30/2022, with panelists Kyle Miskell (Provost Office), Karen Hollebrands (CED) and Alyson Wilson (ORI/COS).
- Member of the planning committee for the second NCSU Equity Research Symposium, Talley Student Union, March 8, 2023.
 - Co-organized and co-moderated the Symposium's opening plenary event: "Equity in Research" with Erin Sills, a panel with Lisa Bass, (College of Education), Melanie Simpson (Molecular and Structural Biochemistry), Caren Cooper (Forestry and Environmental Resources).
- Member of Selection Committee for 2022 Alumni Distinguished Research Award and for membership in the Research Leadership Academy (six awardees selected).
- Solicit nominees for 2023-24 Chair-Elect.

2021-2022

NCSU Research Leadership Academy.

- Elected 2021-22 Chair-Elect and 2022-23 Chair.
- Planning of University Research Symposium and other RLA activities for 2021, 2022, 2023.
- Member of the planning committee for the inaugural NCSU Equity Research Symposium, Talley Student Union, February 8, 2022.
 - Co-organized and moderated the Opening Plenary Panel "Framing Equity" with Julie Ivy and Cranos Williams.
- Member of Selection Committee for 2022 and 2023 Alumni Distinguished Research Award and membership in the Research Leadership Academy.
- Solicit nominees for 2022-23 Chair-Elect.

Panelist (invited) for "Faculty Connections." New Faculty Research Orientation, hosted by the Office of Research and Innovation, Talley Student Center, 3/22/2022.

2020-2021

Dean's Search Committee for CBE Department Head, 2019-2021.

University Faculty Scholars, Nominee Selection Committee, College of Engineering, Member, 2020-21.

Goodnight Early Career Innovator Award, Nominee Selection Committee, College of Engineering, Member, 2021.

Co-organizer and Co-chair, RLA Lunch and Learn: Continuing Our Research During COVID-19, Research Leadership Academy, 9/11/2020.

Supported the organizing committee for the 2021 University Research Symposium of the NCSU Research Leadership Academy, "Climate Change and Resilience" (had been postponed to March 2021 from 2019-20, where I had been one of the three 2019-20 organizing committee members).

2019-2020

Organizing committee for the 2020 University Research Symposium of the NCSU Research Leadership Academy, "Climate Change and Resilience," March 25, 2020 (postponed to 2020-21).
Dean's Search Committee for CBE Department Head, 2019-2020.
COE Doctoral Scholar of the Year, CBE Nominee-Selection Committee member, 2020.
University Faculty Scholars Nominations Committee, College of Engineering, Member, 2019.

2018-2019

COE Committee for Curricula Review, department representative.

2017-2018

Member, Research Computing Committee, University.

2016-2017

Member, Research Computing Committee, University.
NC State Institutional Representative, AIChE RAPID Process Intensification proposal.
Member, Advisory Council, NCSU Data Science Initiative.
Working group on Combustion Research, co-founder. Campus Combustion-Research Poster event, 11/2016.

2015-2016 (Scholarly Leave in France and U.K.)

Member, Research Computing Committee, University.
Member, Advisory Council, NCSU Data Science Initiative.

2014-2015

Member, Advisory Council, NCSU Data Science Initiative.
Member, Research Committee, College.
Member, Research Computing Committee, University.
Member, IT Strategic Plan Process Steering Team.

2013-2014

Member, Research Committee, College.
Member, Research Computing Committee, University.
Member, IT Strategic Plan Process Steering Team.

2012-2013

Member, Research Committee, College.
Member, Research Computing Committee.
Member, IT Strategic Plan Process Steering Team.
NSF Nanomanufacturing internal-preproposal review panel.

2011-2012

Member, Research Committee, College.
Session facilitator, "EPA-RTP Visits NCSU Agenda," University (2/15/2012).
Participant, Selection committee for cluster-hire proposals on Data-Driven Science and on Meso-Engineering, Image Analysis and 4-d Microscopy, University.
Panel chair, New Faculty Orientation, University (August 2011).

2010-2011

Member, Research Committee, College.

2009-2010

Member, Research Committee, College (NCSU).
IGERT internal-preproposal review panel.
Extension Service internal review committee, University.

2005-2006 (University of Massachusetts Amherst)

Chair, Tang Endowment Lecture Series committee, College.

2004-2005

Chair, Tang Endowment Lecture Series committee, College.

Member, Chemical and Environmental Management System Committee, University.

Member, Search Committee for Director of Libraries, University.

Freshman Orientation academic adviser (Summer 2005).

2003-2004

Chair, Tang Endowment Lecture Series committee, College.

Guest judge, ECE Senior Design Projects, College.

Freshman Orientation academic adviser (Summer 2004).

ELab II building dedication committee, College.

2002-2003

Member, Search Committee for Vice Chancellor of Research, University.

Chair, Tang Endowment Lecture Series committee, College.

Freshman Orientation academic adviser (Summer 2003).

2001-2002

Chemical Hazards Committee, University.

Chair, Tang Endowment Lecture Series committee, College.

Freshman Orientation academic adviser (Summer 2002).

2000-2001

Chemical Hazards Committee, University.

Freshman Orientation academic adviser (Summer 2001).

1999-2000 (On sabbatical)

1998-99

Chemical Hazards Committee, University.

Student Evaluations of Teaching committee, College.

Dean's Steering Committee for Campaign UMass "Faculty/Staff Capital Campaign."

Freshman Orientation academic adviser (Summer 1999).

1997-98

Publications Committee, College of Engineering.

Chemical Hazards Committee, University.

Freshman Orientation academic adviser (Summer 1998).

1996-97

Publications Committee, College of Engineering.

Chemical Hazards Committee, University.

Freshman Orientation academic adviser (Summer 1997).

1995-96

Publications Committee, College of Engineering.

Chemical Hazards Committee, University.

Co-author: E. Blunt-Harris, D. Boisclair, J. Clark, L. Craker, S. DiNardi, D. Hoagland, J. Meyer, P. Morgan, M. Rausch, D. Robinson, P. Samal, L. Schwartz, V. Steinberg, M. Weinberg, E. Westhead, and P. Westmoreland, *Laboratory Health and Safety Manual*, University of Massachusetts Amherst (1995).

Departmental and laboratory presentations for spring Open Houses of College.

Invited presentation on "Applying Molecular and Materials Modeling for Chemical Engineering" for University Research Computing Symposium, 10/27/95.

Freshman Orientation academic adviser (Summer 1996).

1994-95

Publications Committee, College of Engineering.

Chemical Hazards Committee, University.

Departmental representative at Dean's Advisory Council lunch and breakfast.

Laboratory presentations for fall and spring Open Houses of College.

Freshman Orientation academic adviser (Summer 1995).

1993-94

Member of Search Committee for Chairman, Electrical and Computer Engineering.

Publications Committee, College of Engineering.

Chemical Hazards Committee, University.

Laboratory presentations for two spring Open Houses of College.

1992-93 [Sabbatical]

1991-92

Freshman Orientation academic adviser (Summer 1992).

Coordinate AIChE activities for Freshman Majors Night, Engineers' Week, Open House.

Nominated and presented Outstanding Woman in Engineering award (Patty Restrepo).

1990-91

Freshman Orientation academic adviser (Summer 1991).

Conducted chemical engineering laboratory tours for College of Engineering Open House.

Nominated and presented Outstanding Woman in Engineering award (Janet Beloin).

1989-90

Freshman Orientation academic adviser (Summer 1990).

Nominated and presented Outstanding Woman in Engineering award (Stephanie Simmons).

1988-89

Freshman Orientation academic adviser (Summer 1989).

College of Engineering Curriculum Committee.

Community College Day presentation.

Nominated and presented Outstanding Woman in Engineering award (Angelina Phelan).

1987-88

Freshman Orientation academic adviser (Summer 1988).

College of Engineering Curriculum Committee.

Community College Day presentation.

Minority Engineering Program - Overview presentation of chemical engineering during orientation.

Contribution to 1988 "Yield Enhancement Brochure" of University Admissions Office.

Nominated and presented Outstanding Woman in Engineering award (Molly Silvestrone).

1986-87

Freshman Orientation academic adviser (Summer 1987).

Nominated and presented Outstanding Woman in Engineering award (Priscilla Robinson).

IV.D. Department

2024-2025

Chair, Diversity/Equity/Inclusion Committee (2021-2024).

Coordinated "Diversity Minute" presentations, LGBTQ+ briefings for ChE 702 and possibly ChE 395, assisted Michael Dickey in contacts for HBCU visits, led re-articulation of the committee's name.

Prepare award nomination packages for 2024 "Early Career Investigator" Award, AIChE Catalysis and Reaction Engineering Division (Milad Abolhasani; successful); 2025 Robert A. Augustine Award, Organic Reactions Catalysis Society (Milad Abolhasani; unsuccessful); 2025 ACS Sustainable Chemistry & Engineering Lectureship Award (Milad Abolhasani; successful); 2025 Alumni Distinguished Research Award and Research Leadership Academy (Milad Abolhasani; under consideration).

Participate in departmental "Future Leaders" event, general grad-recruiting activities, ChE 702 review committees (3), UG Professors and Students luncheon, graduation and seminar events, judge for Schoenborn Symposium.

2023-2024

Chair, Diversity/Equity/Inclusion Committee.

Coordinated "Diversity Minute" presentations, LGBTQ+ briefings for ChE 702 and possibly ChE 395, assisted Michael Dickey in contacts for HBCU visits, led re-articulation of the committee's name.

Vice Chair of 2023-4 Faculty Search Committee with Michael Dickey.

375+ applications, 20+ Zoom interviews, co-hosted four on-campus interview visits.

Prepare award nomination packages for 2023 Rutherford Aris Award, International Society of Catalysis and Reaction Engineering (Milad Abolhasani; unsuccessful) and 2023 AIChE CAST Himmelblau Award (Matthew Cooper et al.; successful).

Participate in departmental "Future Leaders" event, general grad-recruiting activities, ChE 702 review committees (3), graduation and seminar events.

Member, Vivian T. Stannett Fellow Award selection committee.

Organized Class of 1973 reunion as part of the CBE Centennial Gala.

2022-2023

Chair, Diversity/Equity/Inclusion Committee.

Organized faculty/staff DEI activity at August 2022 Faculty Retreat.

With the committee, developed "Diversity Minute" for the faculty meetings and presentation to graduate recruits, and developing an REU proposal focused on HBCU students.

Co-Chair of 2022-3 Faculty Search Committee with Milad Abolhasani.

350 applications, 22 Zoom interviews, 8 on-campus interview visits.

Prepare award nomination packages for Milad Abolhasani (2023 Rutherford Aris Award - unsuccessful, International Society of Catalysis and Reaction Engineering - unsuccessful) and Matthew Cooper et al. 2023 (AIChE CAST Himmelblau Award - successful).

Participate in departmental "Future Leaders" event, general grad-recruiting activities, ChE 702 review committees (3), graduation and seminar events.

2021-2022

Chair, Diversity/Equity/Inclusion Committee.

Collected action suggestions, worked with the committee to revise the department mission statement and create a 2022 CBE DEI Action Plan.

Present with committee to the department Alumni Advisory Committee, 4/29/2022.

Organized June 13, 2022, training workshop.

Participate in departmental "Future Leaders" and general grad-recruiting activities.

Prepare award nomination packages for Milad Abolhasani: AIChE Langer Prize, AIChE Catalysis and Reactor Engineering Division Flytzani-Stephanopoulos Early Investigator Award, AIChE Environmental Division, Early Investigator Award; and for Fanxing Li, ACS Sustainability Lecturer.

AIChE Southeastern Regional Student Conference, hosted virtually by NC State: Composed answers and questions for ChE Jeopardy and served as a judge, judged ChE Car poster competition.

2020-2021

Member, Department Head Search Committee (2019-2021).
Chair, Vivian T. Stannett Fellow Award selection committee.
Judge, Senior Design Day, May 2021.
Participate in departmental "Future Leaders" and general grad-recruiting activities

2019-2020

Member, Department Head Search Committee (2019-2021).
Organizer, Faculty-to-Faculty lunch briefings.
CBE Nominee-Selection Committee member for COE Doctoral Scholar of the Year, 2020.
Chair, Vivian T. Stannett Fellow Award selection committee.
Participate in departmental "Future Leaders" and general grad-recruiting activities

2018-2019

Organizer, Faculty-to-Faculty lunch briefings.
Member, CBE Leadership Review Committee.
Participate in departmental "Future Leaders" and general grad-recruiting activities

2017-2018

Organizer, Faculty-to-Faculty lunch briefings.
Chair, RPT committee for reappointment review of Stefano Menegatti, Fall 2017.
Member, ABET Transport subcommittee.
Praxair TA Award selection committee, Department, Fall 2017.
Chair, Vivian T. Stannett Fellow Award selection committee.
Schoenborn Symposium Award selection committee, January 2018.

2016-2017

Organizer, Faculty-to-Faculty lunch briefings.
ABET Transport subcommittee.
Praxair TA Award selection committee, Department, Fall 2016.

2015-2016

Member, ABET Transport subcommittee.
Ph.D. Preliminary Examinations.
Praxair TA Award selection committee, Department, Spring 2016.

2014-2015

Co-Chair, Faculty Search Committee.
Chair, Department Awards Committee.
Member, ABET Transport subcommittee.
COE Research Committee representative.
Ph.D. Preliminary Examinations.

2013-2014

Chair, Department Awards Committee.
Member, ABET Transport subcommittee.
COE Research Committee representative.
Ph.D. Preliminary Examinations.

2012-2013

Member, ABET Transport subcommittee.
COE Research Committee representative.
Ph.D. Preliminary Examinations.

2011-2012

Ph.D. Preliminary Examinations.
Member, ABET Transport subcommittee.
COE Research Committee representative.

2010-2011

Ph.D. Preliminary Examinations.
Member, ABET Transport subcommittee.
COE Research Committee representative.
Faculty Search Committee, member.

2009-2010 (NC State)

Ph.D. Preliminary Examinations.
Member, ABET Transport subcommittee.

2008-2009 (UMass Amherst, on IPA leave)

Departmental Distinguished Lecturer Committee, member.

2007-2008 (UMass Amherst, on IPA leave)

Departmental Distinguished Lecturer Committee, member.

2006-2007 (UMass Amherst, on IPA leave)

Departmental Distinguished Lecturer Committee, member.

2005-2006 (UMass Amherst)

Outreach coordinator: Web, newsletter, alumni relations.
Tang Lecture Committee representative.

2004-2005

Acting Department Head.
Tang Lecture Committee representative.

2003-2004

Acting Department Head.
ELab II Building Dedication Committee.
Tang Lecture Committee representative.

2002-2003

Graduate Program Director.
Chair, Departmental Personnel Committee.
Faculty Search Committee.
Chair, Search Committee for Laboratory and Facilities Manager.
Outreach coordinator.
Web-page revisions committee.
Building Committee.
Tang Lecture Committee representative.

2001-2002

Chair, Faculty Search Committee.
Chair, Departmental Personnel Committee.
Outreach coordinator.
Building Committee.
Tang Lecture Committee representative.

2000-2001

Graduate Program Director.
Recruit new students.
Administer procedures and provide counsel for current students.
Outreach coordinator.
Personnel Committee, member.
Building Committee.

1999-2000 [Away on sabbatical]

Building Committee.

1998-99

Chair, Ph.D. Qualifying Examinations.
Outreach coordinator.
Building Committee.
Departmental representative to University Chemical Hazards Committee.

1997-98

Graduate Recruiting Committee.
Outreach coordinator.
Departmental contact, Council for Chemical Research.
Monitor departmental Web pages, provide corrections.
Submit articles to Campus Chronicle and News Office on Doherty, Haensel, Malone, Tsapatsis, Watkins.
Departmental representative to University Chemical Hazards Committee.
Member, Building Committee.

1996-97

Graduate Program Director.
Recruit new students.
Administer procedures and provide counsel for current students.
Supervise Graduate Seminar program and T.A. assignments.
Maintain and revise departmental World-Wide Web pages.
Department Head search committee.
Departmental representative to University Chemical Hazards Committee.
Building Committee.

1995-96

Graduate Program Director.
Recruit new students.
Administer procedures and provide counsel for current students.
Supervise Graduate Seminar program and T.A. assignments.
Building Committee.
Develop and maintain departmental World-Wide Web pages.
Departmental representative to University Chemical Hazards Committee.

1994-95

Graduate Program Director.
Recruit new students.
Administer procedures and provide counsel for current students.
Prepare T.A. assignments and coordination.
Develop the initial World-Wide Web pages for the department, including on-line Graduate Brochure.
Revise Graduate Regulations.
Supervise Graduate Seminar program.
Building Committee.
Departmental representative to University Chemical Hazards Committee.

1993-94

- Personnel Committee, chair.
- Prepared faculty evaluations.
- Initiated committee effort to review and promote junior-faculty development.
- Prepared nomination for Val Haensel for Chancellor's Distinguished Teaching Award (successful).
- Faculty Search Committee, member.
- Departmental representative to University Chemical Hazards Committee.

1992-93 [Sabbatical]

1991-92

- Faculty Search Committee, member.
- AICHE Student Chapter advisor.
- Nominated three students who received Outstanding Senior Service Awards from the College.
- Prepared "Primary Elements" article published in *AChExtra* (national student-member magazine) featuring Randy Lavigne.
- Coordinated AIChE activities for Freshman Majors Night, Engineers' Week, Engineering Open House.
- Solicited funds for improvement of undergraduate unit-operations laboratory.
- Prepared successful nomination (Patty Restrepo) for Outstanding Woman in Engineering award.

1990-91

- Solicit funds for improvement of undergraduate unit-operations laboratory.
- Chair and organize content of 1991 Kinetics and Reaction Engineering qualifying examinations.
- Conducted chemical engineering laboratory tours for College of Engineering Open House.

1989-90

- Organize content of 1990 Kinetics and Reaction Engineering qualifying examinations.
- CHE 420 course outline and polymerization-experiment description for curriculum revision.
- Prepared successful nomination for Outstanding Woman in Engineering award (Jackie Hurtle).

1988-89

- Departmental Seminar coordinator.
- Faculty Search Committee member.
- Computer Committee, member.
- Public-relations coordination (News releases, contributions for *Engineering News*).
- Organize content of 1989 Kinetics and Reaction Engineering qualifying examinations.
- Prepared successful nomination for Outstanding Woman in Engineering award (Angelina Phelan).

1987-88

- Departmental Seminar coordinator.
- Faculty Search Committee, member.
- Computer Committee, member.
- Public-relations coordination (News releases, contributions for *Engineering News*).
- Organize content of 1988 Kinetics and Reaction Engineering qualifying examinations.

1986-87

- Library representative.
- Curriculum-revision working group.
- Public-relations coordination (News releases, contributions for *Engineering News* and College information booklet, revised brochure for Polymer Process Engineering Group, Applied Technology Center.)
- Prepared successful nomination for Outstanding Woman in Engineering award (Priscilla Robinson).