

Curriculum Vitae

Michael T. Klein

Present Position

Dan Rich Chair of Energy
Department of Chemical and Biomolecular Engineering
Energy Institute
University of Delaware
Newark, DE 19716

Education

Sc.D. Chemical Engineering, 1981
Massachusetts Institute of Technology

B.Ch.E. Chemical Engineering (with distinction and highest honors), 1977
University of Delaware

Major Research Interests

Upgrading and conversion of renewable and fossil fuels
Chemical Reaction Engineering
Detailed kinetic modeling of complex reaction systems

Experience

7/2010-present	Dan Rich Chair of Energy, Chemical and Biomolecular Engineering University of Delaware
7/2010 - 9/2016	Director, University of Delaware Energy Institute
9/98 - 7/2010:	Board of Governors Professor of Chemical Engineering Rutgers, The State University of New Jersey
9/98 - 7/2008:	Dean and Board of Governors Professor of Chemical Engineering Rutgers, The State University of New Jersey
9/94 - 8/98:	Elizabeth Inez Kelley Professor of Chemical Engineering University of Delaware
7/91 - 6/96:	Chairman, Department of Chemical Engineering University of Delaware
9/89 - 8/94:	Professor of Chemical Engineering University of Delaware
9/88 - 6/91:	Director, Center for Catalytic Science and Technology University of Delaware
2/87 - 9/88:	Associate Dean, College of Engineering University of Delaware
9/85 - 9/89:	Associate Professor of Chemical Engineering University of Delaware
2/81 - 8/85:	Assistant Professor of Chemical Engineering University of Delaware
1/80 - 6/80:	Instructor (Chemical Reaction Engineering) Massachusetts Institute of Technology

Awards, Honors and Scholarly Appointments

Tupras Research and Development Center Advisory Board, November 2016
Saudi Aramco Visiting Professor, King Fahd University of Petroleum and Minerals, October, 2016
2013 Peter H. Given Lectureship in Coal Science, Feb.18-22, 2013
2012-present, Member of the AspenTech Academy
2015-present, Chair of the AspenTech Academy
2011, ACS Fellow
2008 R. H. Wilhelm Award in Chemical Reaction Engineering, AIChE
Editor-in-Chief, *Energy and Fuels*, January 2002 – present
Board of Governors Professor of Chemical Engineering, Rutgers University, 1998-2010
Chair, International Advisory Board, Curtin Centre for Advanced Energy Science and Engineering, Curtin University of Technology, Australia
Participation in Chinese Government “Plan 111”
“Top 100” author in citations in Industrial and Engineering Chemistry
Blue-Green Seminar, University of Michigan and Michigan State University, 10/14/2004
Outstanding Alumnus Award, College of Engineering, University of Delaware, 1998
Elizabeth Inez Kelley Professor of Chemical Engineering, 1994
Presidential Young Investigator Award, National Science Foundation, 1985
ACS Delaware Section Award, 1993
Advisory Board Member, CUNY Department of Chemical Engineering
Associate Editor, *Energy and Fuels*, January 1992-2001
Consulting Editor, *AIChE J.*, January 1992-2002
McGraw-Hill Advisory Committee for Chemical Engineering, 1992-2002.
Editorial Advisory Board for *Encyclopedia of Chemical Processing*, 2001.
Editorial Board for *Reviews in Process Chemistry and Engineering*
International Editorial Board for *Encyclopedia of Catalysis*, 2008.
Reaction Engineering Topical Editor for *Encyclopedia of Catalysis*
Associate Editor, *Industrial and Engineering Chemistry, Fundamentals*, September 1982-83.
Outstanding Young Men of America, 1988
Who's Who in Science and Engineering
Who's Who in Engineering
American Men and Women of Science, 1994
Zeisberg Award for Senior Thesis, Honorable Mention
Who's Who in America
Who's Who in the East

Membership in Professional and Honorary Societies

American Institute of Chemical Engineers
American Chemical Society
Sigma Xi, American Association for the Advancement of Science
Tau Beta Pi, Phi Beta Phi, Omicron Delta Kappa

Professional Activities

National and International Committees

Organizing committee member, 9th Heavy Oil Symposium, Beijing, May 24-25, 2016
Member, Advisory Council, University of New Mexico Center for Emerging Energy Technologies, 2013
Panelist, DOE Bioenergy Research Center Program Reverse Site Review, October 2013
Panelist, GCEP Proposal Review, Stanford University, April 23, 2012
Executive Committee Member, AIChE Center for Energy Initiatives

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Panelist, Review Committee for DOE Carbon Capture Simulation Initiative
Panelist, DOE Bioenergy Research Center Program Reverse Site Review
Search Committee for the Director, American Chemical Society Office of Research Grants and Petroleum Research Fund
Panelist, Department of Energy Workshop on Basic Research Needs in Catalysis, Fossil Fuels Panel, Bethesda, MD, August 2007
Director, AIChE Kinetics, Catalysis and Reaction Engineering Division, 2001-2004.
Director, AIChE Fuels and Petrochemicals Division, 2001-2004.
15th International Symposium on Chemical Reaction Engineering (ISCRE), Program Committee, 1998
13th International Symposium on Chemical Reaction Engineering (ISCRE), Program Committee, 1994
Co-chair (with Jan Lerou, DuPont) Engineering Foundation Conference on Reaction Engineering, February 1993
Director, AIChE Division 20, Kinetics, Catalysis and Reaction Engineering, 1995-96.
Division of Petroleum Chemistry, ACS, Program Committee, 1993
Reaction Engineering Subcommittee, AIChE, 1990
Programming Committee, AIChE Area Ib, Kinetics, Catalysis and Reaction Engineering, 1981-1995
AIChE 1989 National Nominating Committee

Programming at Meetings of Professional Societies

8th Sino-US Conference on Chemical Engineering, Energy Session Chair, Shanghai, China, October 12-15, 2015
8th Symposium on Heavy Petroleum Fractions: Chemistry, Processing and Utilization, Scientific Committee, October 22-24, 2014, Beijing, China
Chairman of the Scientific Committee, 4th International Conference on Biorefinery--Towards Bioenergy, December 3-5, 2013, Xiamen, China
Co-Chair, Session on Clean Utilization of Fossil Oils, 7th Sino-US Joint Chemical Engineering Conference, Beijing, October 13-17, 2013.
Co-Chair, Symposium in Honor of Michael Siskin, 2012 Storch Award, 244th American Chemical Society National Meeting & Exhibition, Philadelphia, PA, August 19-23, 2012.
Technical Committee, Petroleum Phase Behavior and Fouling Conference Petrophase 2012, St. Petersburg, FL June 2012
Technical Committee, The 6th Sino-US Joint Conference of Chemical Engineering, Session 1-A: Clean Utilization of Fossil Energy, November 7, 2011
Technical Committee, Petroleum Phase Behavior and Fouling Conference Petrophase 2011, London, UK July 2011
Organizing Committee and Conference Overview Speaker, Creating the Clean Energy Economy, Clayton Hall, December 2010
Organizing Committee and Treasurer, Petroleum Phase Behavior and Fouling Conference, New Jersey/New York, June 2010
Scientific Committee for the International Biorefinery Conference 2009, Syracuse NY
Co-Chairman, Symposium in Honor of Kenneth B. Bischoff, AIChE Annual Meeting, Salt Lake City, UT, Nov 2007.
Co-Chairman, Symposium on Computer Modeling in Fuel Chemistry, ACS National Meeting, Chicago, August 2001.
Chairman, Tutorial on Molecular Modeling in Refinery Processes, AIChE National Meeting, Houston, March 2000.
Co-Chairman, Symposium on Modeling for On-Line Optimization, AIChE National Meeting, Houston, March 1999.

- Co-Chairman, Symposium on Chemistry of Reactive Intermediates and Modeling in Hydrocarbon Conversion, ACS National Meeting, New Orleans, Fall 1999.
- Co-Chairman, Symposium on Hydroprocessing Options for Meeting Future Transportation Fuel Specifications, AIChE National Meeting, New Orleans, March 1998.
- Co-Chairman, Symposium on *Catalysis in Fuel Processing and Environmental Protection*, ACS National Meeting, Las Vegas, NV, September 1997.
- Co-Chairman, Symposium on *Modeling for On-Line Optimization of Refinery Processes*, AIChE Spring Meeting, Houston, TX, March 1997.
- Vice-Chairman, Symposium I, II & III on *Reaction Engineering*, AIChE National Meeting, New Orleans, LA, February 1996
- Vice-Chairman, Symposium on *Catalytic Conversion of PNA Hydrocarbons*, ACS National Meeting, Chicago, IL, August 1995
- Vice-Chairman, Symposium on *Reaction Path Analysis*, AIChE Annual Meeting, St. Louis, MO, November 1993
- Co-chairman, 205th National ACS Meeting, Division of Petroleum Chemistry, *Resid Upgrading*, 1993
- Chairman, Symposium on *Reactions in Supercritical Fluids*, AIChE Annual Meeting, Miami Beach, FL, November 1992
- Vice-Chairman, Symposium on *Reaction Path Analysis*, AIChE Annual Meeting, Miami Beach, FL, November 1992
- Chairman, Symposium on *Molecular Modeling of Petroleum Processes and Catalysis*, San Francisco, CA, April 1992
- Chairman, Symposium on *Reactions in Supercritical Fluids*, AIChE Annual Meeting, Los Angeles, CA, November 1991
- Vice-Chairman, Symposium on *Reaction Path Analysis*, AIChE Annual Meeting, Los Angeles, CA, November 1991
- Vice-Chairman, Symposium on *Advances in Hydrocracking*, AIChE Annual Meeting, Los Angeles, CA, November 1991
- Chairman, Symposium on *Selectivity in Catalysis*, American Chemical Society Annual Meeting, New York City, NY, August 1991
- Chairman, Symposium on *Synthetic Macromolecules*, American Chemical Society National Meeting, Atlanta, GA, April 1991
- Chairman, *Reactions in Supercritical Fluid Solvents*, AIChE Annual Meeting, Chicago, IL, November 1990
- Chairman, *Reaction Pathway Analysis: Methods*, AIChE Annual Meeting, Chicago, IL, November 1990
- Vice Chairman, *Reaction Pathway Analysis: Applications*, AIChE Annual Meeting, Chicago, IL, November 1990
- Vice-Chairman, *Advances in Hydrocracking*, AIChE Annual Meeting, San Francisco, CA, November 1989
- Vice-Chairman, Symposium on *Reactions in and with Supercritical Fluid Solvents*, AIChE Annual Meeting, Washington, DC, November 1988
- Vice-Chairman, Symposium on *Reaction Pathways: Fundamental Aspects*, AIChE Annual Meeting, New York, November 1987
- Vice-Chairman, Symposium on *Reaction Pathway Fundamentals*, AIChE Annual Meeting, Miami Beach, FL, November 1986
- Chairman, Symposium on *Chemical and Mathematical Modelling of Complex Reaction Systems*, Annual Meeting of the ACS, Anaheim, CA, September 1986
- Chairman, Symposium on *Fundamental Reaction Pathways*, Annual Meeting American Institute of Chemical Engineers, Chicago, IL, November 1985
- Chairman, Symposium on *Pyrolysis and Biomass*, American Chemical Society National Meeting, Miami, FL, April 1985

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- Chairman, Symposium on *Thermal Reaction Pathway Fundamentals*, 1983 AIChE Annual Meeting
- Vice-Chairman, Symposium on *Chemical Pathways in Coal Conversion*, AIChE National Meeting, Houston, TX, March 1983
- Vice-Chairman, Symposium on *Fundamentals of Thermal Reaction Pathways*, AIChE Annual Meeting, Los Angeles, CA, November 1982

Invited Lectures

- Software Tools for Molecular-level Kinetics Modeling of Refinery and Petrochemical Reactors, 26th Annual Saudi-Japan Symposium, King Fahd University of Petroleum and Minerals, November 7-8 2016
- Software Tools for Molecular-level Kinetics Modeling of Refinery and Petrochemical Reactors, King Fahd University of Petroleum and Minerals, Center of Research Excellence in Petroleum Refining & Petrochemicals, October 24, 2016
- Software Tools for Molecular-level Kinetics Modeling of Refinery and Petrochemical Reactors, Saudi Aramco, October 24, 2016
- Software Tools for Reaction Modeling at the Molecular Level, UOP, April 2016
- University of Utah, Chemical Engineering, April, 2016
- Software Tools for Reaction Modeling at the Molecular Level, AspenTech Shanghai Office, October 15, 2015
- Molecular-Level Kinetic Modeling in Refining: Software Tools and their Applications, Sinopec, October 21, 2014
- Molecular-Level Kinetic Modeling in Refining: Software Tools and their Applications, Petrochina, October 20, 2014
- Aspen Tech Webinars, through 2014
- Molecule-based Modeling of Heavy Ends in Refining, RIPP-SINOPEC, March 2014
- Molecular-Level Kinetic Modeling in Refining: Software Tools and Their Applications, RIPP-SINOPEC, March 2014
- Keynote lecture "Transitive Closure: Enabling Atomically Explicit Kinetics Models in Refinery-Wide Modeling" at The 7th Sino-US Joint Conference of Chemical Engineering, 14-18 October, 2013, Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China, with Craig A. Bennett, Zhen Hou and Linzhou Zhang.
- Plenary lecture "Chemical Modeling of Coal Liquefaction" at the International Conference on Coal Science & Technology, September 29 – October 3, 2013
- Keynote talk "Software Tools for the construction of detailed kinetic models" in the ACS Symposium on "**Frontiers in energy conversion and fuel production**", 246th ACS meeting (Indianapolis, September 8-12, 2013)
- Software Tools for the Construction of Detailed Kinetic Models, Catalysis Club of Philadelphia, May 9, 2013
- Plenary Lecture, Infrastructure-Ready Biomass-Derived Oils: Incentives, Options and Process Models, Inaugural Fraunhofer - Delaware Technology Summit, March 5, 2013
- Atom-explicit Molecular Models of Structure and Reactions: BPO HDT, BP, Naperville, IL, January 24, 2013
- The Composition Model Editor, BP, Naperville IL, January 24, 2013
- 2013 Peter H. Given Lectureship in Coal Science: Software Tools for the Construction of Detailed Kinetic Models, February 18, 2013
- 2013 Peter H. Given Lectureship in Coal Science: Chemical Modeling of Direct Coal Liquefaction, February 21, 2013
- Advanced Molecular Modeling of Complex Hydrocarbon Systems, MAGLAB Energy Workshop, Florida State University, November 7-8, 2012
- Modeling the Structure and Reactions of Heavy Oil, JPEC, October 19, 2012, Tokyo, Japan

Modeling the Structure and Reactions of Heavy Oil, International Conference on Chemistry of Heavy Petroleum Fractions and its Impacts on Refining Processes, Beijing, China, October 23, 2012.

ExxonMobil, March 20, 2012

Molecule-based Modeling of Complex Reaction Systems, University of Massachusetts, October 25, 2011

Integrating Biofuels and Petroleum Refining: The Guidance of Quantitative Kinetics and Process Modeling (with Richard Quann), New Industrial Chemistry and Engineering Workshop on Catalysis and Alternative Feedstocks in the Biofuels Industry, September 21-22, Newark, DE

Keynote Lecture, First International Conference on Clean Energy, Dalian, China, April 2011

Florida High Tech Jobs and Economic Development Symposium, April 2011

Florida State University, April 2011

University of Oklahoma, April 2011

BP Molecular Modeling Workshop, March 2011

AIChE Delaware Local Section, February 2011

Lehigh University, February 2011

Pacific Northwest National Laboratory, February 2011

Molecular Modelling of Refinery Processes, Haldor-Topsoe Catalysis Forum, Copenhagen, August 2010.

Conference Keynote Address, Petrophase 2010, June 2010

University of Delaware Energy Institute, Building Kinetic Models, Research Programs and Academic Units in Support of Sustainable Energy Options, February 1, 2010

Participant, Panel on Direct Coal Liquefaction, IFP-Lyon, February 8, 2010

Modeling Lignin Structure and Pyrolysis, Sino-Australian Symposium on Advanced Coal and Biomass Utilisation Technologies, Wuhan, CN, December 2009.

Keynote Lecture, Statistical and Discrete Methods for Modeling Complex Reaction Systems, Sino-AIChE Meeting, Beijing, CN, October 14, 2009

Keynote Lecture, The Composition Modeling Editor Tool for Estimating Properties of Complex Feeds, International Symposium on Value Chain of Heavy Oil: Research to Reality, Beijing, CN, October 14, 2009

Molecular Level Modeling Approaches for the Kinetics of Complex Reaction Systems, Research Institute of Petroleum and Petrochemicals, Sinopec, Beijing, CN, October 15, 2009

Molecule-Based Modeling of Heavy Hydrocarbon Structure and Reactions: Discrete and Statistical Approaches, BP, Naperville, IL, August 27, 2009

Keynote Lecture, Molecule-Based Modeling of Heavy Hydrocarbon Structure and Reactions: Discrete and Statistical Approaches, North American Meeting of the Catalysis Society, San Francisco, CA, June 10, 2009

Modeling Lignin Structure and Pyrolysis, ExxonMobil, Clinton, NJ, September 30, 2008

Attribute-Based Modeling of Heavy Hydrocarbon Structure and Reactions, Chinese National Meeting on Heavy Hydrocarbon Conversion, Xiamen, China, November 2007

Molecule-Based Modeling of Heavy Hydrocarbon Structure and Reactions: Discrete and Statistical Approaches, Chinese University of Petroleum, Beijing, China, November 2007

Detailed Kinetic Modeling of Complex Reactions: Chemistry, Software and IT Issues, Chinese University of Petroleum, Beijing, China, November 2007

Molecule-Based Modeling of Heavy Hydrocarbon Structure and Reactions: Discrete and Statistical Approaches, Chicago Catalysis Club, October 8, 2007

Detailed Kinetic Modeling of Complex Reactions: Chemistry, Software and IT Issues, UOP, Des Plaines, IL, October 9, 2007

Molecule-Based Modeling of Heavy Hydrocarbon Structure and Reactions: Discrete and Statistical Approaches, ExxonMobil Research, August, 2007

Keynote Lecture, Kinetic Modeling Approaches and Software Tools, NASCRE-2, Houston, TX
7Feb07

The Chemical Reaction Engineering of Microreactors, Corning, NY, Dec 2005.

Young Faculty Forum, AIChE National Meeting, November 2005

Microkinetic Modeling, SABIC, Riyadh, Kingdom of Saudi Arabia, June 2005

Microkinetic Modeling for Process Optimization, AspenWorld 2004, Orlando, Florida

Sunoco, EO MicroKinetic Modeling, May 5, 2004

Detailed Kinetic Modeling of Complex Reactions: Chemistry, Software and IT Issues, GE Global
Research, Irvine, CA, March 2004.

Aspen Technology (UK)/Ibn Sina-SABIC, January 2004

Microkinetic Modeling of Hydrocarbon Reduction, Wiesbaden, Germany, May 2003

Detailed Kinetic Modeling of Complex Reactions, Corning, Inc. Corning NY, March 2003

Detailed Kinetic Modeling of Complex Reactions, City College of New York, March 2003

Microkinetic Modeling, Aspen Technology, October 2002

Microkinetic Modeling, Rohm and Haas, November 2002

ExxonMobil, October 2001

The Transition from Department Chair to Dean, AIChE Annual Meeting, Indianapolis, IN,
November 2002.

Automated Kinetic Model Building NCUT, Alberta Canada June 2002.

Modeling Catalytic Hydrocracking: A Mechanistic Foundation, Plenary Lecture, Session on
Kinetics and Mechanisms of Petroleum Processes, ACS National Meeting, Chicago, August
2001.

Topical Initiatives in Support of the Engineering Core: An Engineering Information Technology
Example," The New Jersey Section of the AIChE, April 10, 2001.

Initiatives-Driven Development of Programs in Engineering, Rutgers University, April 10, 2001.

Topical Initiatives in Support of the Engineering Core: An Engineering Information Technology
Example," The Ceramic Association of New Jersey, March 2001.

Applications of Technology to Chemical Mixtures, Conference sponsored by Colorado State
University, January 11, 2001.

Henry E. Bent Distinguished Lecture Series, University of Missouri-Columbia, March 1, 2001

Imperial College London, October 2000

UOP, Chicago, October 2000

Northwestern University, April 2000

NJIT, March 2000

AspenWorld 2000, February 2000

The Catalysis Society of Metropolitan New York, January 2000

Phillips Petroleum Company, September 1999

Shell Chemical Company, August 1999

John Dickinson High School Commencement Address, June 1999

Ciba Specialty Chemicals, September 1998

Convocation Address, Rutgers College of Engineering, May 21, 1998

UOP Workshop on Detailed Kinetic Modeling, March 1998

UOP, December 1997

AspenWorld 97, Boston, MA, October 1997

Rutgers University, October 1997

University of California, Los Angeles, February 1997

University of California, Berkeley, February 1997

Iowa State University, April 1997

Shell Chemical Company, October 1996

DuPont Company, February 1996

UOP, 1995

Chevron USA, 1995

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Engineering Foundation Meeting, Reaction Engineering V, October 1995
Fourteenth North American Meeting of the Catalysis Society, Snowbird, Utah, June 1995
Exxon, May 1995
Chevron USA, November 1994
UOP, November 1994
Gordon Conference on Hydrocarbon Resources, Hawaii, November 1994
Purdue University, September 1994
Argonne/Amoco Hydrocarbon Chemistry Program, Distinguished Seminar Series Speaker,
August 1994
American Chemical Society, Division of Petroleum Chemistry Award Symposium, (in honor of
T. F. Yen) "Monte Carlo Simulation of Asphaltene Structure, Reactivity and Reaction," San
Diego, March 1994.
University of Michigan, March 1994
The Pennsylvania State University, April 1993
Princeton University, February 1993
University of Hawaii, January 1993
New Jersey AIChE, Fall Lecture Series, November 1992
University of Maryland, October 1992
University of Alberta, September 1992
Mobil Research and Development, May 1992
Massachusetts Institute of Technology, May 1992
Koninklijke/Shell, Amsterdam, The Netherlands, April 1992
University of Wisconsin, April 1992
Michigan State University, February 1992
Phillips Petroleum, November 1991
Lehigh University, Bethlehem, PA, April 1991
ARCO Symposium, New Frontiers in Catalysis, Newtown Square, PA, October 1990
Department of Energy, Catalyst Testing Workshop, Pittsburgh, PA, September 1990
Koninklijke/Shell, Amsterdam, The Netherlands, March 1990
Mobil Workshop on Chemical Reactions in Complex Systems, March 1990
Exxon Research and Engineering, Florham Park, NJ, March 1990
"Monte Carlo Simulation of Complex Reaction Systems: A Vehicle for Catalyst Design"
Engineering Foundation Conference on "Chemical Reaction Engineering III," Santa Barbara,
CA, February 1990
General Electric, January 1990
Ciba-Geigy, McIntosh, Alabama, November 1989
Phillips Petroleum, April 1989
Texaco, April 1989
Ciba-Geigy, Mobile, Alabama, December 1988
City College of New York, November 1988
Rutgers University, 1990
Yale University, November 1988
Amoco Oil Company Quarterly Technical Meeting, Invited Outside Speaker,
November 1988
Exxon Research and Engineering (Florham Park, NJ), August 1988
Massachusetts Institute of Technology, April 1988
Research Needs in Coal Pyrolysis, ARCO, Newtown Square, April 1988
Amoco Performance Products, Inc., December 1987
Mobil (Princeton) Research and Development, January 1988
Amoco Oil, January 1988
Exxon Corporate Research and Development (Clinton), August 1987
Sun Oil, April 1987

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University of Massachusetts, Amherst, MA, March 1987
AAAS National Meeting, Philadelphia, PA, May 1986
Eastman Kodak Co., Rochester, NY, April 1986
University of Minnesota, Minneapolis, MN, April 1986
Stevens Institute of Technology, Hoboken, NJ, March 1986
USDA Forest Products Laboratory, January 1986
Exxon Engineering and Research Co., Annandale, NJ, November 1985
Phillips Petroleum, Bartlesville, OK, November 1985
Dow Chemical Company, Freeport, TX, September 1985
Louisiana State University, Baton Rouge, LA, April 1985
Cornell University, Ithaca, NY, April 1985
Mobil Paulsboro Laboratories, March 1985
Maryland Section AIChE, February 1985
Chicago Catalysis Society, January 1985
Pacific Basin Chemical Society International Meeting, Honolulu, HI, December 1984
Amoco Oil Company, Naperville, IL, May 1984
University of Pennsylvania, February 1984
Participant in National Science Foundation-sponsored workshop, "Biomass Engineering: Thermochemical Conversion Research Needs," Kona, HI, October 1983
The Standard Oil Company (OHIO), September 1983
FACSS Tenth Annual Meeting, "Lignin Pyrolysis Mechanisms," Phila., PA, September 1983
Gordon Conference on Analytical Pyrolysis, "Lignin Pyrolysis Mechanisms as Discerned Through Model Compound Reaction," July 1983
University of Notre Dame, March 1983
Delaware Valley Section AIChE, "Chemicals From Wood," March 1983
University of Delaware, The Honors Program Undergraduate Science and Engineering Seminar, "Chemicals and Fuel From Coal," September 1982

Presentations at Professional Meetings

1. Mayuresh Sahasrabudhe, Chandra Saravanan, Scott R. Horton, Zhen Hou, Pratyush Agarwal, Juan Lucio-Vega and Michael T. Klein, Enhancing the Value of Detailed Kinetic Models through the Development of Interrogative Software Applications Triveni Billa, AIChE National Meeting, November 2016.
2. Pratyush Agarwal, Juan Lucio-Vega, Scott R. Horton and Michael T. Klein, Molecular-Level Kinetic Model Informed Life Cycle Analysis of Green Diesel Production, AIChE National Meeting, November 2016.
3. Molecular-Level Simulation of Thermogravimetric Analysis (TGA): A Cellulose Pyrolysis Example, Juan Lucio-Vega, Scott R. Horton and Michael T. Klein, AIChE National Meeting, November 2016.
4. Data Auditing: Analysis Techniques for the Compatibility of Experimental Data for Molecular-Level Kinetic Models, Scott R. Horton, Triveni Billa, Pratyush Agarwal, Juan Lucio-Vega, Mayuresh Sahasrabudhe, Saru Saravan and Michael T. Klein, AIChE National Meeting, November 2016.
5. Introducing petroleomics into molecule-based kinetic models, Pacificchem 2015, Honolulu, Hawaii, December 2015.
6. Molecular-Level Kinetic Modeling in Thermochemical Conversions: Software Tools and Their Applications, AIChE Annual Meeting, Salt Lake City Utah, November 2015
7. Software Tools for Molecular-Level Kinetic Modeling in Thermochemical Conversions, Eighth Sino-US Conference on Chemical Engineering, Shanghai, China, October 2015
8. Molecular-Level Kinetic Modeling in Thermochemical Conversions: Software Tools and Their Applications, ACS National Meeting, Boston, August 2015.

9. Analyzing Refinery Unit Kinetic Models by Reaction Network Visualization, ACS National Meeting, Boston, August 2015.
10. Keynote: Molecular-Level Kinetic Modeling in Biomass Thermochemical Conversions: Software Tools and Their Applications, 249th ACS National Meeting, Denver, Colorado, March 22-26, 2015.
11. Atom-Explicit Composition Models of Heavy Oils, with Zhen Hou, Linzhou Zhang, Triveni Billa, and Scott Horton, Heavy Oil Meeting, Beijing, October 2014.
12. *with* Quach, A. L. and Moreno, B. M., Discrimination between Free-Radical and Concerted Mechanisms in Hydrocarbon Pyrolysis, Fourth International Conference on Biorefinery, Xiamen, China, December 3-5, 2013.
13. Modeling Resid Structure, 14th International Conference on Petroleum Phase Behavior and Fouling, Rueil-Malmaison, France, 10-13 June 2013 (S. Zhao, speaker)
14. Molecular-level kinetic modeling of resid thermolysis, 14th International Conference on Petroleum Phase Behavior and Fouling, Rueil-Malmaison, France, 10-13 June 2013 (S. Horton, speaker)
15. Molecular-Level Modeling of Municipal Solid Waste Gasification, Innovations of Green Process Engineering for Sustainable Energy and Environment Session, Scott R. Horton*, Michael T. Klein and Francis P. Petrocelli, AIChE Annual Meeting, San Francisco, CA 2013
16. Molecular-Level Composition Model for Heavy Petroleum Resid Supercritical Fluid Extraction Fractions Linzhou Zhang*, Zhen Hou, Triveni Billa, Scott R. Horton, Michael T. **Klein**, Zhiming Xu, Quan Shi, Suoqi Zhao and Chunming Xu, AIChE Annual Meeting, San Francisco, CA 2013
17. Modeling Biomass-to-Fuels Processing Brian M. Moreno* and Michael T. **Klein**, AIChE Annual Meeting, San Francisco, CA 2013
18. Molecular-Level Modeling of Municipal Solid Waste Gasification, Scott R. Horton*, Yu Zhang, Craig A. Bennett, Michael T. **Klein** and Frank Petrocelli, AIChE Annual Meeting, San Francisco, CA 2013
19. Toward Transitive Closure in Refinery-Wide Modeling: Atomically Explicit Kinetics Models Craig A. Bennett*, Zhen Hou, Linzhou Zhang and Michael T. **Klein**, AIChE Annual Meeting, San Francisco, CA 2013
20. Automated Molecular Level Composition Modeling for Complex Hydrocarbon Mixtures, Zhen Hou*, Linzhou Zhang, Triveni Billa, Scott R. Horton and Michael T. **Klein**, AIChE Annual Meeting, San Francisco, CA 2013
21. Automating Molecular Modeling of Gasification with the Kinetic Modelers Toolbox, Craig A. Bennett, Scott R. Horton*, Michael T. Klein and Francis P. Petrocelli, AIChE Annual Meeting, Pittsburgh, PA 2012
22. MOLECULAR MODELING FOR ULTRA-DEEP HYDRODESULFURIZATION OF LIGHT GAS OIL, Kazuhiko Hagiwara, Shogo Teratani, Ryuzo Tanaka*, Michael T. Klein, Craig A. Bennett, Zhen Hou, 244th American Chemical Society National Meeting & Exhibition, Philadelphia, PA, August 19-23, 2012.
23. Composition modeling of heavy petroleum oil, 2012 Storch Award Symposium in honor of Dr. Michael Siskin 244th American Chemical Society National Meeting & Exhibition, Philadelphia, PA, August 19-23, 2012.
24. "Mechanistically informed pathway kinetic model for the Fischer-Tropsch wax hydrocracking," Simone Gamba*, Craig A. Bennett, Michael T. Klein, and Laura A. Pellegrini, 244th American Chemical Society National Meeting & Exhibition, Philadelphia, PA, August 19-23, 2012.
25. "Automating Molecular Modeling of Resid Pyrolysis," 13th International Conference on Petroleum Phase Behavior and Fouling, St. Petersburg Beach, Florida, June 10-14, 2012.
26. "Using Mechanistically Informed Pathways to Control the Automated Growth of Reaction Networks," 2011 Sino-Australian Symposium on Advanced Coal and Biomass Utilisation Technologies, Wuhan, China, December 10, 2011

27. "Molecule-based modeling of the structure and reactions of complex feed stocks," The 6th Sino-US Joint Conference of Chemical Engineering, Session 1-A: Clean Utilization of Fossil Energy, November 7, 2011
28. "Tools for Molecule-Based Modeling of Biomass Structure and Reaction," Michael T. Klein, Brian M. Moreno, & Hannah R. Kempton, 242nd ACS National Meeting & Exposition: Computational Methods, Modeling, and Simulations in Fuel and Energy Technologies, August 28, 2011, Denver, CO
29. "Modeling Heavy Hydrocarbon Structure and Reaction," Zhen Hou, Craig Bennett and Michael T. Klein, 242nd ACS National Meeting & Exposition: Computational Methods, Modeling, and Simulations in Fuel and Energy Technologies, August 31, 2011, Denver, CO
30. "Statistical Approaches for Modeling Complex Petroleum Systems," Pacificchem meeting, December 2010.
31. "Software tools for modeling the thermochemical conversion of lignin to chemicals and fuels," Pacificchem meeting, December 2010.
32. "Solvent Effects on Reactions in Supercritical Fluids", AIChE Annual Meeting, Salt Lake City, UT, November 2010.
33. *with* Concetta LaMarca, Characteristics of optimal chain transfer solvents for heavy hydrocarbon conversion, ACS National Meeting, Boston, August 2010.
34. *with* Bennett, C. B., Hou, Z., Kim, C. J., Moreno, B. M., Building Complex Kinetics Models with INGen, 239th ACS National Meeting, San Francisco, CA March 21-25, 2010.
35. "Colleagues in the Development of Kinetic Modeling Approaches and Software Tools", AIChE Annual Meeting, Nashville, TN, November 2009.
36. *with* Bennett, C. B., Hou, Zhen, "Matthew Neurock's Linking of Petroleum Resids and Quantum Chemistry", AIChE Annual Meeting, Philadelphia PA, November 2008.
37. *with* Bennett, C. B., Hou, Zhen and Darin M. Campbell, "Molecule-Based Modeling of Heavy Hydrocarbon Structure and Reactions: *Discrete and Statistical Approaches*", ACS Annual Meeting, Philadelphia PA, August 2008.
38. *with* Bennett, C. B., Hou, Zhen, "Detailed Kinetic Modeling: Reaction Network and Parameter Estimation Issues," AIChE Annual Meeting, Salt Lake City, November 2007.
39. Ryuzo Tanaka (speaker), Michael T. Klein, Wei Wei, Craig A. Bennett, and Gang Hou, "Molecule-Based Kinetic Modeling of Combined Cat Feed Hydrotreating-FCC," ACS 229th National Meeting, San Diego, CA, March 14, 2005
40. *with* Wei, W. S. Shah, C. Bennett and M. T. Klein, Jr., "Tools for Editing Detailed Kinetic Models: A Catalytic Reforming Example," ACS 228th National Meeting, Philadelphia, PA, August 25, 2004
41. Structure Reactivity Relationships in Hydroprocessing, ACS 227th National Meeting, Anaheim, CA March 29, 2004.
42. *with* Wei, W., "KMT - Kinetic Modeling Toolbox and Its Applications," AIChE National Meeting, San Francisco, CA, 2003
43. *with* Wei, W., "KMT - Software Tools for the Construction of Detailed Kinetic Models for Complex Reactions," ACS National Meeting, New York, NY, 2003
44. *with* Wei, W. and Nandoliya, S., "Kinetic Modeling Software for Reforming," ACS Spring Meeting, Orlando, FL, 2002
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223. Molecular-Level Kinetic Modeling of Resid Pyrolysis, Scott R. Horton, Linzhou Zhang, Zhen Hou, Craig A. Bennett, Michael T. Klein and Suoqi Zhao, *Ind. Eng. Chem. Res.*, **2015**, 54 (16), pp 4226–4235.
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228. Virk, P. S. and Klein, M. T., Frontier Orbital Interpretation of Gas Release Pathways in Lignin Thermolysis, *Energy Fuels*, **2016**, 30 (10), pp 8043–8046.

Books and Monographs

- Klein, M. T., Hou, G., Broadbelt, L. J., Kumar, A., Bertolacini, R. J. "Molecular Modeling in Heavy Hydrocarbon Conversions," Taylor & Francis, 2006.
- Song, C.S., M. T. Klein, B. Johnson and J. Reynolds. *Catalysis in Fuel Processing and Environmental Protection*. Elsevier, Amsterdam (as volume 50 of a serial publication *Catalysis Today*), March **1999**, 172 pp.
- Song, C.S., M. Klein and J. Reynolds. *Catalytic Conversion of Polycyclic Aromatic Compounds*. Elsevier, Amsterdam (as volume 31 of a serial publication *Catalysis Today*), September **1996**, 188 pp.

Funded Research

Proposal	Title	Amount
1	Elucidation of Lignin and Lignite Pyrolysis Pathways and Mechanisms, University of Delaware Research Foundation, January 1981.	\$10,000
2	Reaction Engineering Analysis of the Hydrocracking of Heavy Oil Feedstocks, (with B. C. Gates), Sun Tech, February 1982,	\$149,112
3	Modification of Lignin Thermolysis Toward Optimal Hydrogen Utilization, National Science Foundation, May 1982.	\$52,898
4	Enhanced Coal Liquefaction by Hydrolysis in Supercritical Fluids, with M. E. Paulaitis and A. B. Stiles, Department of Energy, Aug. 1982.	\$249,984
5	Lignin-Derived Chemicals for Adhesives: Depolymerization of Lignin by Thermolysis in Supercritical Fluids USDA Forest Products Laboratories.	\$20,000
6	Enhanced Thermochemical Conversion of Lignin to Chemicals by Selective Catalytic Hydrodeoxygenation, National Science Foundation, Aug. 1984.	\$103,575
7	Determination of Chemical Reaction Pathways and Mechanisms Relating to Heavy Resource Upgrading in Supercritical Solvents, The Standard Oil Co. (Ohio), Dec. 1984.	\$48,755
8	Enhanced Coal Liquefaction by Pyrolysis in Supercritical Fluids, with M. E. Paulaitis and S. I. Sandler, Department of Energy, Sept. 1985.	\$174,958
9	Catalysis of High Temperature Fragmentation Reactions in and with Supercritical Fluid Solvents, American Chemical Society, Petroleum Research Fund, Sept. 1985.	\$35,000
10	Identification and Manipulation of the Initial Reaction Pathways and Mechanism of Direct Coal Liquefaction, Amoco Oil Company (\$500,000) and State of Delaware Research Partnership Program (\$100,000), Dec. 1987-1992	\$600,000
11	Hydrocracking Reaction Pathways and Kinetics, Sun Oil, Graduate Student Fellowship, Jan. 1988.	\$48,000
12	A Chemical Modelling Analysis of the Thermal Stability of High-Performance Polymers, Amoco/Delaware Research Partnership Program (1988-91)	\$283,540
13	Presidential Young Investigator Award, NSF Funding (1985-89)	\$312,500
14	Industrial Matching For PYI Award:	
15	Amoco Oil (1985, 1986)	\$30,000
16	Standard Oil (1985, 86, 87)	\$18,500
17	Hercules (1986, 1987)	\$15,000
18	ICI (1986)	\$5,000
19	Mobil (1986)	\$5,000
20	Fundamentals of Hydrocracking Aromatic and Naphthenic Compounds: The Basis of Computational Chemical Engineering Analysis, Mobil Oil Company, 1/1/89 - 6/1/92	\$200,000
21	Design, Synthesis and Characterization of Novel, Fine-Particle Unsupported Catalysts for Coal Liquefaction (with H. C. Foley), Department of Energy, 9/26/90 - 9/25/93	\$370,000

22	Resolution of the Reaction Fundamentals Underlying Heavy Oil Conversion Alternative: The Chemical Modelling Methodology, British Petroleum America, 6/1/89 - 5/31/93	\$256,000
23	Selective Catalytic Reduction of NOx in Presence of Oxygen (with A. B. Stiles), Columbia Gas/Delaware Research Partnership, 5/11/90 - 6/30/92	\$342,000
24	Reaction and Reactor Analysis Involving High Temperature Water (with T. B. Brill), Army Research Office/University Research Initiative, 7/1/92 - 6/30/1995	\$1,708,319
25	Thermal Cracking in Petroleum Processes, Exxon Education Foundation (1991, 1992, 1993)	\$30,000
26	Chemical Engineering and the Environment: Advanced Instrumentation Requirements, UNIDEL Foundation (with several ChE Faculty colleagues) (1991-1999)	\$300,000
27	Parallel Processing Supercomputing Initiative, UNIDEL Foundation 1/20/89-12/31/99	\$600,000
28	Stability of Advanced Composites and Related Materials: Kinetics and Mechanisms of Nitrile Hydrolysis at Severe Conditions, Du Pont (\$120,000)/-Delaware Research Partnership (\$45,000)	\$165,000
29	Chemical Modelling Analysis of Polyamides, Amoco Performance Products (\$45,000)/Delaware Research Partnership, 12/19/91 - 12/18/92	\$90,000
30	New Chemical Information Technology: Reaction Models with 'On the Fly' Computational Chemistry, Mobil (\$25,000)/Delaware Research Partnership (\$25,000), 7/92-6/93	\$50,000
31	ASSERT Award for "Explosive and Energetic Functional Group Chemistry in Supercritical Water" (with T. B. Brill), Army Research Office, 9/93-8/96	\$105,000
32	Managing the Information in Integrated Manufacturing Processes through Molecule-based Models, BP America and Delaware Research Partnership, 7/1/93-12/31/93	\$40,000
33	Preliminary Evaluation of the Kinetics of Coal Liquefaction Resid Conversion (with W. H. Calkins and H. Huang), Subcontract from CONSOL under DOE Contract, 4/15/93 - 9/1/93	\$19,500
34	New Chemical Information Technology: Reaction Models with 'On the Fly' Computational Chemistry, Mobil/Delaware Research Partnership, 7/93-6/94	\$42,000
35	Study of Short Contact Time Direct Coal Liquefaction Using a Novel Batch Reactor, Department of Energy, 9/93-8/96	\$200,000
36	Molecular Modeling of Cracking Chemistry, BP America (\$25,000) and Delaware Research Partnership (\$25,000)	\$50,000
37	Molecule-Based Information Technology for Integrated Manufacturing, Mobil/Delaware Research Partnership, 7/94-6/95	\$50,000
38	A Study of the Conversion of the Non-distillable Portion (Resid) of Coal Liquefaction Process Streams and Correlation of Conversion Reactivity with Resid Structure, CONSOL/DOE Contract, 8/94-4/97	\$106,642
39	Management of Aromatics Usage in Fluid Catalytic Cracking, W. R. Grace, 12/94-11/95	\$35,000

40	Graph Theory as a Basis for Building Chemical Information Technology, Exxon/Delaware Research Partnership, 12/94-11/95	\$70,000
41	Graph Theory as a Basis for Building Chemical Information Technology Modeling of the Kinetics of Catalytic Isomerization and Cracking, 12/94-11/95	\$50,000
42	Computer Generated Design and Analysis Tools for Plant Optimization: The Construction of a Hydrocracking Kinetics Model Builder, Chevron/Delaware Research Partnership, 9/95-8/98	\$180,000
43	Development of a Coke Drum Kinetics Model for the Prediction of Product Yields and Properties, BP, 7/95-6/96	\$25,000
44	The Hydrocracking Reaction Pathways, Kinetics and Mechanisms of Long-Chain Alkyl Aromatics, Mobil, 7/95-6/96	\$25,000
45	Construction of a Molecular Representation of a Complex Feedstock by Monte Carlo and Quadrature Methods, M. W. Kellogg, 7/95-6/96	\$5,000
46	Computer Generated Kinetic Modeling: The Construction of a Partial Oxidation Kinetics Model, DuPont Company, 4/96-9/96	\$5,000
47	The Construction of a Molecular Representation of Asphaltene Structure by Monte Carlo Method, Mobil, 4/96-3/97	\$40,000
48	Managing the Flow of Aromatics in Refinery Streams, UOP, 2/96-2/97	\$50,000
49	Measurements of the Kinetics of Ethylene Hydrogenation with Fe ₂ O ₃ and Fe ₂ O ₃ - (C ₂ H ₅) _x AL Catalysts, Union Carbide, 4/96-3/97	\$24,560
50	Hydrocracking Long-Chain Alkyl Polynuclear Aromatics: Reaction Pathways, Kinetics and Mechanisms, Mobil Technology Company, 11/96-10/97	\$25,000
51	Study of Solvent and Catalyst Interactions in Direct Coal Liquefaction, U. S. Department of Energy, 9/97-5/2000.	\$200,000
52	Computer-Assisted Modeling of Catalytic Reforming," UOP/Delaware Research Partnership, 2/97-2/98.	\$54,000
53	Chemical Plant Safety Models: The Dynamics of Exothermic Hydroisomerization Reactions, Mobil/Delaware Research Partnership.	\$86,000
54	Software for the Computer-Generated Construction of Chemical Process and Kinetics Models, Chevron/Delaware Research Partnership, 9/97-8/98.	\$100,000
55	Estimation of Asphaltene Reaction Products by Analytical Reaction Chemistry, Mobil 3/98-2/99.	\$33,000
56	The Thermodynamics of Polynuclear Aromatics Saturation Reactions, Mobil Technology Company, 5/31/98-8/31/98.	\$10,000
57	Kinetic Measurements and Modeling of Hydrothermal Conditions, National Science Foundation, 7/1/98-6/30/01 (with Prof. T. Brill).	\$400,000
58	Developing a Predictive Strategy for Chemical Mixtures, NIH/NIEHS, 7/1/98-6/30/03, (with Dr. Raymond Yang, CSU).	\$1,688,404
59	Support for Chemical Kinetics and Catalysis, Shell Chemical Company, 5/28/98-10/28/98.	\$13,000

60	The Design of Additive Technologies for the Minimization of Acetaldehyde Formation from PET, Ciba Specialty Chemicals Corporation, 1998-99.	\$125,907.60
61	KMAST Membership Support (UOP, BP, Petrobras, RIPP)	\$50,000.00
62	Rutgers (MTK sole PI) Subcontract via Virginia Tech, Novel Fast Pyrolysis/Catalytic Technology for the Production of Stable Upgraded Liquids, US Department of Energy, with S. Ted Oyama (PI), Foster Agblevor and Francine Battaglia, 2008-2010.	\$79,395.00.
63	Predicting Coal-biomass Gasification using Experiments and Detailed Chemical Reaction Kinetics, Virginia Tech-US DOE.	\$236,998.00
64	Modeling Lignin Pyrolysis Feeds, Reactors and Product Kinetics, SDSU	\$170,991.00
65	Collaboration and exchange between the China University of Petroleum and the University of Delaware	\$120,000
66	Molecule-based Modeling of Catalytic Reforming Reaction Kinetics, RIPP-Sinopec, 11/9/2011-11/8/2013	\$318,781
67	The Development of a Kinetic Modeler's Toolbox for JPEC, Japan Petroleum Energy Center, 10/19/2011 - 3/31/2017	\$135,000
68	Modeling the Plasma Gasification of Municipal Solid Waste: An Air Products-University of Delaware Energy Institute Collaborative Project, Air Products and Chemicals, Inc., 10/15/2011 - 9/30/2015,	\$343,995
69	Uncertainty in the Estimates of Molecular Composition from Limited Data, MIT/BP, 4/1/2012 - 11/30/2014,	\$215,748
70	Air Liquide - UDEI 4 Year Collaborative Agreement, America Air Liquide, 11/17/2011 - 12/31/2015,	\$400,000
71	Kinetic Models for Hydroprocessing Petroleum-Biocrude Blends - A Basis for Process Development and the Identification of Technology Gaps, BP International Limited, 12/1/2011 - 11/30/2012,	\$75,066
72	CCR-Platforming Micro-Kinetics Model Development, Reliance Industries, Limited, June 2014-June 2015	\$150,000,
73	Molecule-based Modeling of Continuous Catalytic Reforming Reaction Kinetics, Sinopec, 7/14/14-6/13/15	\$176,316
74	Developing a Detailed Alkylation Model, RIPP/Sinopec, 9/1/15-8/31/17	\$460,636
75	Detailed Mechanistic Kinetic Model Development for Hydrotreating/Hydrocracking/Isomerisation Including Catalyst Deactivation and Catalyst Properties, Reliance Industries, 1/1/2016-12/31/2017	\$402,636
76	SusChEM: Biobased Platform for the Sustainable Molecular Design and Controlled Synthesis of Block Polymers from Renewable Feedstocks, with Thomas H. Epps III (PI), NSF, 5/1/15-4/30/18	\$497,809
77	Joint Project on the Modeling of Heavy Petroleum Molecular Conversion, PetroChina, 7/1/16-9/30/17	\$150,961
78	Investigation of Coal-Biomass Catalytic Gasification Using Experiments, Reaction Kinetics, and Computational Fluid Dynamics, Virginia Tech/DOE-10/1/2010-9/30/2015	\$236,998
79	Advancing Coal Catalytic Gasification to Promote Optimum Syngas Production, Virginia Tech/DOE, 10/1/2014-7/31/2017	\$109,614

80	Chemical Reaction Modeling of Biomass Conversion via Tail Gas Reactive Pyrolysis, USDA, 1/10/2016-1/9/2017	\$12,577
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Research Student Supervision

PhD

1. PETROCELLI, Francis P., "Chemical Modeling of the Thermal and Catalytic Depolymerization Lignin" (June 1985)
2. BOGAERT, Ricardo J., "Chemical Vapor Deposition of Amorphous Silicon Films from Disilane" (June 1986) (with T. W. Fraser Russell)
3. McDERMOTT, John Brian, "Chemical and Stochastic Modelling of Complex Reactions: A Lignin Depolymerization Example" (August 1986)
4. SAVAGE, Phillip Erwin, "Chemical and Mathematical Modeling of Asphaltene Reaction Pathways" (December 1986)
5. ABRAHAM, Martin A., "Reactions with Supercritical Fluid Solvents of Heteroatom-Containing Model Compounds of Heavy Feedstocks" (June 1987)
6. TRAIN, Peter Michael, "Stochastic and Chemical Modeling of Lignin Liquefaction" (June 1987)
7. ROHR, JR., Donald Frank, "Modelling Reaction and Diffusion in Epoxy-Amine Polymerization Kinetics" (May 1988)
8. TOWNSEND, Susan Holt, "Enhanced Coal Liquefaction by Hydrolysis in Supercritical Fluids" (December 1988)
9. LAPINAS, Tomas, "Catalytic Hydrocracking of Fused-Ring Aromatic Compounds: Chemical Reaction Pathways, Kinetics, and Mechanisms" (May 1989)
10. WU, Benjamin C., "Solvent Effects on Reactions in Supercritical Fluids" (May 1990) (with S. I. Sandler)
11. LANDAU, Ralph N., "Efficient Chemical Modeling of the Hydrocracking of Heavy Oils" (June 1991)
12. PALMESE, Giuseppe, "Origin and Influence of Interphase Material Property Gradients in Thermosetting Composites" (December 1991) (with R. L. McCullough)
13. LAMARCA, Concetta, "Kinetic Coupling in Multicomponent Pyrolysis Systems" (May 1992)
14. LIBANATI, Cristian, "Discrete Modeling of Molecular Events: Stochastic Kinetics and Monte Carlo Simulation of Reaction and Polymer Mobility" (May 1992)
15. NEUROCK, Matthew, "A Computational Chemical Reaction Engineering Analysis of Asphaltene Reaction Pathways" (August 1992)
16. NIGAM, Abhash, "Lumping in the Reaction Modelling of Complex Feedstocks" (August 1992)
17. STARK, Scott, "Parallel Computation in Chemical Reaction Engineering" (August 1992) (with A. Beris)
18. PROVINCE, William, "Investigation of the Initial Reaction Pathways and Mechanisms of Direct Coal Liquefaction" (August 1992)
19. TORRY, Lori A., "Oxidation in Supercritical Water: Experiments and a Low Conversion Model" (October 1992)
20. TRAUTH, Daniel, "Efficient Representation of Residium Structure using Monte Carlo Methods" (June 1993)
21. READ, Carole J., "Reactant and Catalyst Structure/Function Relationships in the Hydrocracking of Biphenyl Moieties" (December 1993)

22. KORRE, Stella, "Quantitative Structure/Reactivity Correlations as a Reaction Engineering Tool: Applications to Hydrocracking of Polynuclear Aromatics" (August 1994)
23. BROADBELT, Linda, "The Thermal Stability of High Performance Polymeric Materials: A Chemical Modelling Analysis" (December 1994)
24. WALTER, Timothy, "Kinetics-Assisted Design of Coal Liquefaction Catalysts" (1995)
25. RUSSELL, Carlonda L., "Hydrocracking of Long-Chain Alkyl-Substituted Polyaromatic Hydrocarbons" (1995)
26. FAKE, Dean, "Design of Optimally Kinetically Coupled Reactions: Emphasis of Real System Complexities" (1995)
27. WATSON, Beth, "Rate Laws Capturing the Kinetic Coupling of Acid Catalysed Cracking Reactions" (1995)
28. WANG, Xiaogong, "Supercritical Water as a Reaction Medium: Remediation of Waste Streams" (1997)
29. IYER, Sada, "Remediation of Hazardous Wastes by Reactions in Supercritical Water" (1997)
30. IZZO, William, "Hydrothermal Reaction of Nitriles: Reaction Pathways, Mechanisms and Kinetics" (1997)
31. CAMPBELL, Darin, "Bimolecular Reactions in Hydrocarbon Conversions" (1997)
32. HARRELL, Cynthia, "Reactions In and With Supercritical Water: Fundamentals and Applications" (1998)
33. JOSHI, Prasanna, "Molecular Modeling of the Catalytic Reforming of Naphtha" (1998)
34. KUMAR, Ankush, "Stochastic Models of Heavy Hydrocarbon Structure and Reactivity" (2000)
35. HOU, Gang, "Mechanism-Based Modeling of Catalytic Hydrocracking" (2001)
36. WEI, Wei, "The Interface of Chemical Engineering and IT in Kinetic Models" (2004)
37. BENNETT, Craig, "User-controlled Kinetic Network Generation with INGen," (2009)
38. Hou, Zhen, "Software Tools for Molecule-Based Kinetic Modeling of Complex Systems," 2011.
39. Brian Moreno, "Thermochemical Conversion of Biomass: Models and Modeling Approaches," 2014
40. Horton, Scott, "Modeling Municipal Solid Waste Gasification: Molecular-level Kinetics and Software Tools," April 2016