

# Curriculum Vitae

## Michael T. Klein

### Present Position

Professor Emeritus  
Department of Chemical and Biomolecular Engineering  
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

<b>7/2010-9/2020</b>	Dan Rich Chair of Energy, Chemical and Biomolecular Engineering University of Delaware
<b>7/2010 - 9/2016</b>	Director, University of Delaware Energy Institute
<b>9/98 - 7/2010:</b>	Board of Governors Professor of Chemical Engineering Rutgers, The State University of New Jersey
<b>9/98 - 7/2008:</b>	Dean and Board of Governors Professor of Chemical Engineering Rutgers, The State University of New Jersey
<b>9/94 - 8/98:</b>	Elizabeth Inez Kelley Professor of Chemical Engineering University of Delaware
<b>7/91 - 6/96:</b>	Chairman, Department of Chemical Engineering University of Delaware
<b>9/89 - 8/94:</b>	Professor of Chemical Engineering University of Delaware
<b>9/88 - 6/91:</b>	Director, Center for Catalytic Science and Technology University of Delaware
<b>2/87 - 9/88:</b>	Associate Dean, College of Engineering University of Delaware
<b>9/85 - 9/89:</b>	Associate Professor of Chemical Engineering University of Delaware
<b>2/81 - 8/85:</b>	Assistant Professor of Chemical Engineering University of Delaware
<b>1/80 - 6/80:</b>	Instructor (Chemical Reaction Engineering) Massachusetts Institute of Technology

### **Awards, Honors and Scholarly Appointments**

2015-present, Chair of the AspenTech Academy  
Executive Advisory Board, AspenTech, April 2019-present  
Saudi Aramco Chaired Visiting Professor, King Fahd University of Petroleum and Minerals  
Editor-in-Chief, *Energy and Fuels*, January 2002 – December 31, 2019  
2013 Peter H. Given Lectureship in Coal Science, Feb.18-22, 2013  
2012-present, Member of the AspenTech Academy  
2011, ACS Fellow  
2008 R. H. Wilhelm Award in Chemical Reaction Engineering, AIChE  
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**

Technical Committee and Treasurer, Petrophase 2020  
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

Chairman, *Reaction Pathway Analysis*, AIChE Annual Meeting, Pittsburgh, 2018  
Chairman, *Reaction Pathway Analysis I*, AIChE Annual Meeting, Minneapolis, October 2017  
Vice Chairman, *Reaction Pathway Analysis II*, AIChE Annual Meeting, Minneapolis, October 2017  
Chairman, *Reaction Pathway Analysis*, AIChE Annual Meeting, San Francisco, CA, November 2016  
8<sup>th</sup> 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, 244<sup>th</sup> 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

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- 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
- 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 Kinetic Modeling of Refinery and Petrochemical Reactors, In Honor of the Wilhelm Award Recipient, AIChE National Meeting, Fall 2019.
- Software Tools for Molecular-level Kinetic Modeling of Refinery and Petrochemical Reactors, George A. Olah Award in Hydrocarbon or Petroleum Chemistry, Monday, April 01, 2019
- Molecule-based Models for Optimizing the Performance of Refinery Units: A Hydrocracking Example, 8th ARRC-JCCP/Idemitsu International Symposium, ADNOC Research Center, February 2019
- Software Tools for Molecular-level Kinetic Modeling of Refinery and Petrochemical Reactors, IFP, February, 2018
- Plenary Lecture, 7<sup>th</sup> Takreer Research Center-JCCP/Idemitsu Refining R&D International Symposium, Software Tools for Molecular-level Kinetic Modeling of Refinery Reactors, Abu Dhabi, September 25-27, 2017.
- Software Tools for Molecular-level Kinetic Modeling of Refinery and Petrochemical Reactors, KBC, July 18, 2017
- Software Tools for Molecular-level Kinetics Modeling of Refinery and Petrochemical Reactors, 26<sup>th</sup> 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 7<sup>th</sup> 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

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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  
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

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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  
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. Software tools for molecular level kinetic modeling in thermochemical conversions, Spring 2019 ACS National Meeting, Orlando, FL, March 31 – April 4, 2019.
2. Software tools for molecular-level modeling of refinery and petrochemical reactors, ACS National Meeting, New Orleans, LA, March 18-22, 2018. Division of Industrial and Engineering Chemistry.

3. State of the Art in Characterizing Complex Hydrocarbon Mixtures, and what to do with it, 2017 AIChE National Meeting, Division Plenary: Imaging of Heavy Hydrocarbon Molecule Structures, October 30, 2017.
4. Pratyush Agarwal and Michael T. Klein, Kinetic Modeling of the Production of Green Diesel Via Hydroprocessing, AIChE Annual Meeting, Minneapolis, MN, October 2017.
5. Pratyush Agarwal and Michael T. Klein, Reducing Molecular-Level Kinetic Models to Decrease Solution Times, ACS National Meeting, Washington D.C., August 2017.
6. Pratyush Agarwal, Juan Lucio-Vega, Kaitlyn Engler, and Michael T. Klein, Molecular-Level Kinetic Modeling of Green Diesel Production Via Hydrodeoxygenation and Hydroisomerization, ACS National Meeting, Washington D.C., August 2017.
7. Modeling lignin pyrolysis reaction mechanisms, Storch Award Symposium, 252nd ACS National Meeting, Philadelphia, PA, Monday, August 22, 2016
8. 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.
9. 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.
10. 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.
11. 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.
12. Introducing petroleomics into molecule-based kinetic models, Pacificchem 2015, Honolulu, Hawaii, December 2015.
13. Molecular-Level Kinetic Modeling in Thermochemical Conversions: Software Tools and Their Applications, AIChE Annual Meeting, Salt Lake City Utah, November 2015
14. Software Tools for Molecular-Level Kinetic Modeling in Thermochemical Conversions, Eighth Sino-US Conference on Chemical Engineering, Shanghai, China, October 2015
15. Molecular-Level Kinetic Modeling in Thermochemical Conversions: Software Tools and Their Applications, ACS National Meeting, Boston, August 2015.
16. Analyzing Refinery Unit Kinetic Models by Reaction Network Visualization, ACS National Meeting, Boston, August 2015.
17. Keynote: Molecular-Level Kinetic Modeling in Biomass Thermochemical Conversions: Software Tools and Their Applications, 249th ACS National Meeting, Denver, Colorado, March 22-26, 2015.
18. Atom-Explicit Composition Models of Heavy Oils, with Zhen Hou, Linzhou Zhang, Triveni Billa, and Scott Horton, Heavy Oil Meeting, Beijing, October 2014.
19. *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.
20. Modeling Resid Structure, 14<sup>th</sup> International Conference on Petroleum Phase Behavior and Fouling, Rueil-Malmaison, France, 10-13 June 2013 (S. Zhao, speaker)
21. Molecular-level kinetic modeling of resid thermolysis, 14<sup>th</sup> International Conference on Petroleum Phase Behavior and Fouling, Rueil-Malmaison, France, 10-13 June 2013 (S. Horton, speaker)
22. 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

23. 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
24. Modeling Biomass-to-Fuels Processing Brian M. Moreno\* and Michael T. Klein, AIChE Annual Meeting, San Francisco, CA 2013
25. 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
26. 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
27. 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
28. 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
29. MOLECULAR MODELING FOR ULTRA-DEEP HYDRODESULFURIZATION OF LIGHT GAS OIL, Kazuhiko Hagiwara, Shogo Teratani, Ryuzo Tanaka\*, Michael T. Klein, Craig A. Bennett, Zhen Hou, 244<sup>th</sup> American Chemical Society National Meeting & Exhibition, Philadelphia, PA, August 19-23, 2012.
30. Composition modeling of heavy petroleum oil, 2012 Storch Award Symposium in honor of Dr. Michael Siskin 244<sup>th</sup> American Chemical Society National Meeting & Exhibition, Philadelphia, PA, August 19-23, 2012.
31. "Mechanistically informed pathway kinetic model for the Fischer-Tropsch wax hydrocracking," Simone Gamba\*, Craig A. Bennett, Michael T. Klein, and Laura A. Pellegrini, 244<sup>th</sup> American Chemical Society National Meeting & Exhibition, Philadelphia, PA, August 19-23, 2012.
32. "Automating Molecular Modeling of Resid Pyrolysis," 13<sup>th</sup> International Conference on Petroleum Phase Behavior and Fouling, St. Petersburg Beach, Florida, June 10-14, 2012.
33. "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
34. "Molecule-based modeling of the structure and reactions of complex feed stocks," The 6<sup>th</sup> Sino-US Joint Conference of Chemical Engineering, Session 1-A: Clean Utilization of Fossil Energy, November 7, 2011
35. "Tools for Molecule-Based Modeling of Biomass Structure and Reaction," Michael T. Klein, Brian M. Moreno, & Hannah R. Kempton, 242<sup>nd</sup> ACS National Meeting & Exposition: Computational Methods, Modeling, and Simulations in Fuel and Energy Technologies, August 28, 2011, Denver, CO
36. "Modeling Heavy Hydrocarbon Structure and Reaction," Zhen Hou, Craig Bennett and Michael T. Klein, 242<sup>nd</sup> ACS National Meeting & Exposition: Computational Methods, Modeling, and Simulations in Fuel and Energy Technologies, August 31, 2011, Denver, CO
37. "Statistical Approaches for Modeling Complex Petroleum Systems," Pacifichem meeting, December 2010.
38. "Software tools for modeling the thermochemical conversion of lignin to chemicals and fuels," Pacifichem meeting, December 2010.
39. "Solvent Effects on Reactions in Supercritical Fluids", AIChE Annual Meeting, Salt Lake City, UT, November 2010.

40. *with* Concetta LaMarca, Characteristics of optimal chain transfer solvents for heavy hydrocarbon conversion, ACS National Meeting, Boston, August 2010.
41. *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.
42. "Colleagues in the Development of Kinetic Modeling Approaches and Software Tools", AIChE Annual Meeting, Nashville, TN, November 2009.
43. *with* Bennett, C. B., Hou, Zhen, "Matthew Neurock's Linking of Petroleum Resids and Quantum Chemistry", AIChE Annual Meeting, Philadelphia PA, November 2008.
44. *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.
45. *with* Bennett, C. B., Hou, Zhen, "Detailed Kinetic Modeling: Reaction Network and Parameter Estimation Issues," AIChE Annual Meeting, Salt Lake City, November 2007.
46. 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 229<sup>th</sup> National Meeting, San Diego, CA, March 14, 2005
47. *with* Wei, W. S. Shah, C. Bennett and M. T. Klein, Jr., "Tools for Editing Detailed Kinetic Models: A Catalytic Reforming Example," ACS 228<sup>th</sup> National Meeting, Philadelphia, PA, August 25, 2004
48. Structure Reactivity Relationships in Hydroprocessing, ACS 227<sup>th</sup> National Meeting, Anaheim, CA March 29, 2004.
49. *with* Wei, W., "KMT - Kinetic Modeling Toolbox and Its Applications," AIChE National Meeting, San Francisco, CA, 2003
50. *with* Wei, W., "KMT - Software Tools for the Construction of Detailed Kinetic Models for Complex Reactions," ACS National Meeting, New York, NY, 2003
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53. *with* Nandoliya, S.; Wei, W.; Bennett, C.; Hou, G.; Broadbelt, L. J., Software Tools for Representing Complex Feed Stocks through Blending Strategies, ACS National Meeting, April 2002
54. *with* Linda J. Broadbelt, Monica A. Mazurek, "Predicting Complex Organic Mixture Atmospheric Chemistry Using Computer-Generated Reaction Models," Presented at the American Geophysical Union, Fall 2001 Meeting, December 10-14, 2001, San Francisco, CA
55. *with* G. Hou, "Mechanistic Kinetic Modeling of Heavy Paraffin Hydrocracking," ACS National Meeting, Chicago, IL, August 2001.
56. *with* G. Hou, "LFER's as Modeling Tools for Parameter Estimation," ACS National Meeting, Chicago, IL, August 2001.
57. Symposium on Understanding Reactivity, "Linear Free Energy Relationships as an Engineering Tool," AIChE Annual Meeting, Los Angeles, CA, November, 2000.
58. *with* G. Hou and Ankush Kumar, "Tutorial on Detailed Kinetic Modeling of Refinery Processes," AIChE National Meeting, Atlanta, GA, March 2000.
59. *with* G. Hou and Ankush Kumar, "Detailed Kinetic Modeling in the Context of Reactor Analysis," AIChE National Meeting, Atlanta, GA, March 2000.
60. *with* G. Hou and Ankush Kumar, "Detailed Kinetic Modeling of Gas Oil HDS," AIChE National Meeting, Atlanta, GA, March 2000.
61. *with* G. Hou, "Model Solving Techniques for Detailed Kinetic Models," AIChE National Meeting, Houston, TX, March 1999.
62. *with* G. Hou, "Automated Molecule-Based Kinetic Modeling of Complex Processes: A Hydroprocessing Application," AIChE National Meeting, Houston, TX, March 1999.

63. Plenary talk, Symposium on Multiscale Reaction and Reactor Modeling, "Mechanistic Kinetic Modeling: Applying Fundamental Chemistries to Complex Processes, AIChE Annual Meeting, Miami Beach, FA, November, 1998
64. *with* A. Kumar, P. V. Joshi, T. I. Mizan, G. Hou, "Use of Stochastic Rules in the Construction of Reaction Models for Fluid Catalytic Cracking" AIChE Annual Meeting, Miami Beach, FA, November 1998
65. *with* A. Kumar, P. V. Joshi, and S. Iyer, "Heavy Hydrocarbon Pyrolysis: An Integrated Approach to Structure and Reaction Modeling," AIChE Annual Meeting, Miami Beach, FA, November 1998
66. *with* T. I. Mizan and G. Hou, "Molecule-Based Hydroprocessing Modeling" AIChE National Meeting, New Orleans, LA, March 1998
67. *with* T. I. Mizan, "Mechanistic Modeling of the Hydroisomerization of High Carbon Number Waxes," AIChE National Meeting, New Orleans, LA, March 1998
68. "Molecule-Based Reaction Engineering: Interfacing Fundamental and Process Chemistry" AIChE National Meeting, New Orleans, LA, March 1998
69. *with* S. D. Brandes, R. A. Winschel, W. H. Calkins, H. Huang, D. Campbell, S. Wang and K. Wang, "The Reactivity of Direct Coal Liquefaction Distillation Resids," 23rd International Technical Conference on Coal Utilization & Fuel Systems, Clearwater, FL, March 1998.
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75. *with* C. L. Harrell, B. Izzo and T. Adschiri, "Hydrolysis of Nitriles at Sub- and Supercritical Conditions: Mechanistic Elucidation," The 4th International Symposium of Supercritical Fluids, Sendai, Japan, May 1997.
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77. *with* S. D. Iyer and P. V. Joshi, "Modeling of Supercritical Water Oxidation of Alcohols," AIChE Annual Meeting, Chicago, IL, November 1996.
78. *with* Broadbelt, L. J. and Grittman, D., "Computer Generated Pyrolysis Models: Applications of Monte Carlo Simulation, Graph Theory, and Quantum Mechanics," 1996 World Congress, San Diego, CA, July 1996.
79. *with* Campbell, D, "Kinetic Modeling and the Quantitative Use of Chemistry in the Study of Complex Reaction Systems," 1996 World Congress, San Diego, CA, July 1996.
80. *with* Izzo, B. (Presenter) and Harrell, C. (Presenter), "Reaction of Nitrile Pollutants in High Temperature Water: Reaction Pathway Analysis and Kinetic Modeling," 1996 World Congress, San Diego, CA, July 1996.
81. *with* P. V. Joshi, "Computer Generated Modeling: Application of Graph Theory," Reaction Engineering V Conference, St. Augustine, FL, October 1995
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83. AIChE Annual Meeting, "Chemical Modeling: The Quantitative Use of Chemistry in the Reaction Engineering Analysis of Complex Reactions Systems," San Francisco, CA, November 1994.
84. *with* Wang, X. (Speaker), "The Destruction of 2-Nitroaniline in Supercritical Water: The Influence of the Temperature and the Density of Water on the Reaction Pathway and Kinetics," AIChE Meeting, Miami Beach, FL, November 1995.
85. *with* Campbell, D. (speaker), "Construction of a Molecular Representation of a Complex Feedstock by Monte Carlo and Quadrature Methods," AIChE Meeting, Miami Beach, FL, November 1995.
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89. *with* Trauth, D. M. (Speaker), S. M. Stark, T. F. Petti, M. Neurock and M. Yasar, "Representation of the Molecular Structure of Petroleum Resid Through Characterization and Monte Carlo Modelling," American Chemical Society, Symposium on Resid Upgrading, Division of Petroleum and Fuel Chemistry, Denver, March 1993.
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91. *with* Walter, T. D. (Speaker), S. M. Casey and H. C. Foley, "The Effects of Iron Carbonyl-based Catalyst Precursors on the Reaction of 4-(Naphthylmethyl)bibenzyl," American Chemical Society, Symposium on Iron-Based Catalysts for Coal Liquefaction, Mechanisms, Division of Fuel Chemistry, Denver, March 1993.
92. *with* L. J. Broadbelt (Speaker) and M. T. Klein, "Mechanistic Modelling of Polymer Pyrolysis Using Monte Carlo Methods," AIChE Annual Meeting, Molecular Modelling for Product Development, Miami Beach, November 1992.
93. *with* L. Torry (Speaker) and M. T. Klein, "Oxidation of Mixtures in Supercritical Water: A Structure/Reactivity Model," AIChE Annual Meeting, Environmental Reaction Engineering, Miami Beach, November 1992.
94. *with* L. Torry (Speaker) and M. T. Klein, "Kinetics and Mechanisms of Reactions in High Temperature Water," AIChE Annual Meeting, High Temperature Processing of Materials, Miami Beach, November 1992.
95. *with* S. C. Korre (Speaker), M. T. Klein and R. J. Quann, "Hydrocracking of Fused-Ring Aromatic and Naphthenic Compounds: Reaction Pathways and Rate Laws," AIChE Annual Meeting, Reaction Path Analysis, Miami Beach, November 1992.
96. *with* S. Stark (Speaker) and M. T. Klein, "Stochastic Reaction Methods for Kinetically Coupled Systems: An Investigation of Parallelization Strategies on MIMD and SIMD Parallel Computers," AIChE Annual Meeting, Parallel Computing, Miami Beach, November 1992.
97. *with* C. L. Russell (Speaker) and M. T. Klein, "Hydrocracking Reaction Pathways, Kinetics and Mechanisms of n-Alkylbenzenes," AIChE Annual Meeting, Miami Beach, November 1992.
98. *with* Gron, L. U. (Speaker), M. A. Barteau and H. C. Foley, "Quantitative *In Situ* Infrared Spectroscopy for the Kinetic Study of Resin-Catalyzed Dehydration of t-Butyl Alcohol," American Chemical Society National Convention, Division of Petroleum Chemistry, San Francisco, April 1992.
99. *with* Walter, T. D., S. M. Casey and H. C. Foley, "Reaction of 4(Naphthylmethyl)Bibenzyl Thermally and in the Presence of  $\text{Fe}(\text{CO})_3(\text{PPH}_3)_2$ ," Proceedings of Liquefaction Contractors' Review Conference, U.S. Department of Energy, Pittsburgh, September 1992.

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101. *with* Read, C. (Speaker), "Reactant Structure/Function Relationships in the Catalytic Hydrocracking of Biphenyl Moieties," 1991 Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, November, 1991.
102. *with* Nigam, A. (Speaker) and M. Neurock, "Reconciliation of Molecular Detail and Lumping: An Asphaltene Thermolysis Example," ACS Symposium on Kinetic and Thermodynamic Lumping of Multicomponent Mixtures, Atlanta, 1991.
103. *with* Nigam, A. (Speaker) and K. B. Bischoff, "Lumping of Discrete Kinetic Systems," ACS Symposium on Kinetic and Thermodynamic Lumping of Multicomponent Mixtures, Atlanta, 1991.
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105. *with* Read, C. (Speaker), and A. T. Lapinas, "Efficient Cleavage of Biphenyl Moieties: A New Reaction Pathway in Catalytic Hydrocracking", 12th North American Meeting of the Catalysis Society, Lexington, KY, May 1991.
106. *with* L. Torry (Speaker), "Oxidation in Supercritical Water: Experiments and a Low Conversion Model," AIChE Annual Meeting, Los Angeles, CA, November 17-22, 1991.
107. AIChE Annual Meeting, "Catalytic Hydrogenation and Hydrocracking of Fluorene: Reaction Pathways, Kinetics, and Mechanisms," San Francisco, CA, November 1989.
108. AIChE Annual Meeting, "Identification and Implications of a Polar Transition State during Hydrolysis in Supercritical Water," Washington, DC, November 1988.
109. ACS Annual Meeting, "Chemical Solvent Effects During Reactions in Supercritical Fluid Solvents," Denver, April 1987.
110. AIChE Annual Meeting, "Chemical Solvent Effects During Reactions in Supercritical Fluid Solvents," Miami Beach, November 1986.
111. AIChE Annual Meeting, "Physical Solvent Effects During Reactions in Supercritical Fluid Solvents," Miami Beach, November 1986.
112. AIChE National Meeting, Chemical Pathways in Coal Conversion Symposium, "Modifying Lignin Pyrolysis by Catalytic Hydrodeoxygenation," Houston, TX, March 31, 1983.
113. AIChE Annual Meeting, Fundamentals of Thermal Reaction Pathways Symposium, "Simulation of Lignin Pyrolysis," Los Angeles, CA, November 1, 1982.
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