

AIChE Centennial: ChE Research and Technology: Past and Future

Topical Conference at the 2008 AIChE Annual Meeting

**Philadelphia, Pennsylvania
16 - 21 November 2008**

ISBN: 978-1-61567-213-4

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2008) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2009)

For permission requests, please contact AIChE
at the address below.

AIChE
3 Park Avenue
New York, NY 10016-5991

Phone: (203) 702-7660
Fax: (203) 775-5177

www.aiche.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

Success and Prospects in Thermodynamics	1
<i>Peter T. Cummings</i>	
Success and Prospects in Transport	2
<i>Morton Denn</i>	
Success and Prospects in Catalysis and Reaction Engineering	3
<i>W. Nicholas Delgass</i>	
Success and Prospects in Process Systems	4
<i>George Stephanopoulos</i>	
Success and Prospects in Bioengineering	5
<i>Harvey W. Blanch</i>	
The Evolution, Structure and Utility of Separations as An Academic Disciplinary Area	6
<i>Judson King</i>	
Membrane Separations-100 Years of Achievements and Challenges	13
<i>Anthony Fane</i>	
Affinity Separations in the Biotechnology Industry	21
<i>Chris Lowe</i>	
ChEmical Engineering and Nuclear Technology at Oak Ridge National Laboratory	22
<i>Robert M. Wham, Phil McGinnis</i>	
ChEmical Engineering and Nuclear Technology at Argonne National Laboratory	23
<i>Ralph Leonard</i>	
A Rich History in Nuclear Materials Processing Technology at Los Alamos National Laboratory	24
<i>Mark Dinehart</i>	
Processes and Experiences at the Hanford Site	25
<i>George Reddick Jr.</i>	
The Role of ChEmical Engineering in the Development and Operation of Nuclear Technologies at the Idaho National Laboratory	32
<i>Jack D. Law, Jack D. Law, Roger N. Henry</i>	
Savannah River National Laboratory – a 30 Year History in the Advancement of Environmental Science and Engineering	33
<i>T. Bond Calloway</i>	
Success and Prospects in Fuels and Energy	34
<i>F. Emil Jacobs</i>	
Success and Prospects in ChEmicals	35
<i>Jeffrey J. Siirola</i>	
Success and Prospects in Food and Consumer Products	36
<i>John Leikhim</i>	
Success and Prospects in Pharmaceutical and Health Care Industry	37
<i>Michael P. Thien</i>	
Success and Prospects in Advanced Materials and Polymers	38
<i>Jocelyn E. Scott</i>	

Recipes, Models, ChEmical Processing and CRE	39
<i>Octave Levenspiel</i>	
ChEmical Reaction Engineering: Looking towards the Future from a Molecular Perspective.....	40
<i>Alexis T. Bell</i>	
Heat Management in ChEmical Reactors-Solved and Unsolved Problems.....	41
<i>Dan Luss</i>	
Polymer Reaction Engineering - Historical Development, Current Vitality and Some Future Challenges.....	44
<i>W. Harmon Ray</i>	
Education Challenges and Opportunities in Pharmaceutical Engineering as An Emerging Academic Discipline.....	45
<i>Piero M. Armenante</i>	
The Changing Role of ChEmical Engineers in R&D in the Pharmaceutical Industry.....	46
<i>Edward Paul, Michael P. Thien</i>	
An Introspective of the Regulatory Influence on Drug Development	47
<i>Christine Seymour</i>	
Quo Vadis Biochemical Engineering?	48
<i>John G. Aunins</i>	
What Can One Do with a New Separation Process?.....	49
<i>Edwin N. Lightfoot</i>	
Advice to a Young Bioseparations Scientist/engineer: Thoughts from a Career	51
<i>Georges Belfort</i>	
Membrane Bioseparations – Look How Far We've Come!.....	52
<i>Andrew Zydney</i>	
History of Insulin Purification	53
<i>Warren MacKellar</i>	
Separations Challenges in Aqueous Separations.....	54
<i>Michael Ladisch</i>	
The Role of Mathematical Programming in the Evolution from Planning and Scheduling towards Enterprise-Wide Optimization.....	55
<i>Ignacio E. Grossmann</i>	
Production Planning and Scheduling, Computer Integrated Manufacturing and Supply Chain Management.....	56
<i>Shinji Hasebe</i>	
Large-Scale Nonlinear Programming: An Integrating Framework for Enterprise-Wide Dynamic Optimization.....	57
<i>Lorenz T. Biegler</i>	
The Evolution, Growth and Future Perspectives of Operations in Process Systems Engineering.....	58
<i>G. V. Reklaitis</i>	
Computational Statistical Mechanics: Past, Present, and Future	59
<i>Glenn H. Fredrickson</i>	
Perspectives on the Past, Present and Future Advances in Computational ChEmistry and Their Application to Catalysis	60
<i>Matthew Neurock</i>	

Thin Films and Nanostructures of Hard Materials: Progress Made and Current Challenges In the Computational Modeling of Their Processing and Function	61
<i>Dimitrios Maroudas</i>	
Polymer-Induced Drag Reduction of Turbulent Flows: What Have We Learnt from Direct Numerical Simulations ?	62
<i>Antony N. Beris, Gaurab Samanta, Kostas D. Housiadas</i>	
Dynamic Models of Biological Systems. A Hotbed for Nonlinear Analysis	63
<i>Doraiswami Ramkrishna</i>	
Paint-by-Numbers: Pattern Formation In Two-Dimensional Sheets of Cells	67
<i>Stanislav Y. Shvartsman</i>	
Three Phases of ChEmical Reaction Engineering.....	68
<i>James Wei</i>	
Bioreaction Engineering: Evolution and Future Needs.....	74
<i>Michael L. Shuler</i>	
Catalysis and Reaction Engineering: Sites, Pellets, and Reactors	75
<i>Enrique Iglesia</i>	
The Evolution of Electrochemical Reaction Engineering and Future Directions	77
<i>Richard Alkire</i>	
Past, Present and Future of Metabolic Engineering	80
<i>Eleftherios Terry Papoutsakis</i>	
Past, Present and Future of Biocatalysis.....	81
<i>Douglas S. Clark</i>	
Past, Present and Future of Drug Delivery.....	82
<i>Nicholas A. Peppas</i>	
Past, Present and Future of Cellular Engineering	83
<i>Larry V. McIntire</i>	
A Century of ChEmical and Physical Adsorption to Characterize Catalysts	84
<i>Burtron H. Davis</i>	
Surface Science and Catalysis of Mixed Metal Oxides	85
<i>Israel E. Wachs, Kamalakanta Routray, Taejin Kim</i>	
Redox Thermodynamics of Ceria and Ceria Mixed Oxides.....	88
<i>Raymond J. Gorte</i>	
Advances In Computational Catalysis: Past, Present and Future.....	89
<i>Matthew Neurock</i>	
An International Assessment of Research in Catalysis by Nanostructured Materials	90
<i>Robert J. Davis</i>	
History of Catalysis: An Industrial Perspective	91
<i>John Armor</i>	
The Complex Science of Catalysis and Catalytic Materials. A Historic and Forward Looking Perspective.....	92
<i>Rutger A. van Santen</i>	
Advances in Catalysis. A Historical Perspective	93
<i>Burtron H. Davis</i>	
Future Directions in Surface Catalysis	94
<i>Bruce C. Gates</i>	

Particle Technology in Early 19th Century Explosive Powder Manufacture	96
<i>Robert Howard, Dan Muir, R. Bertrum Diemer Jr.</i>	
History and Development of Salt Production Processes and Crystals	103
<i>Roma Gimelfarb</i>	
History of Solids Processing at the Dow ChEmical Company	104
<i>Karl Jacob</i>	
Progress toward First-Principles Design of Particle Processes at Merck	105
<i>James N. Michaels</i>	
History of Aerosol Manufacture of Materials	106
<i>Sotiris E. Pratsinis</i>	
The Development and Commercialization of the DuPont Chloride Process for the Manufacture of Pigments Based on Titanium Dioxide.....	107
<i>Austin H. Reid Jr.</i>	
The Interplay Between Simulations and Thernodynamic Models.....	108
<i>Berend Smit</i>	
Perspectives and Prospects for Thermodynamic Modeling	109
<i>Walter G. Chapman</i>	
Predictive Thermochemistry from Quantum ChEmistry: Current State and Perspectives	110
<i>Andreas Klamt</i>	
Simulation of Electrolytes: Model Development and Industrial Practice.....	111
<i>Andre Anderko</i>	
Energy Applications: Impact of Data and Models.....	112
<i>Jefferson Creek</i>	
The Role of Experiments In the Development of ChEmical Technology	120
<i>Joan F. Brennecke</i>	
Development of Air Pollution Law Over the Past 100 Years	121
<i>Mary Ellen Ternes, Lee Paddock</i>	
The 100 Year War: A History of U.S. Air Pollution Science and Policy	129
<i>John Bachmann</i>	
Clean Air Act "Good, Bad, and Room for Improvement"	130
<i>John Dege</i>	
Preparing for Potential Greenhouse Gas Legislation	133
<i>Sunil P. Hangal</i>	
40 Years of Surface Science at Stanford: A Kinetic Perspective	134
<i>Robert J. Madix</i>	
Toward Ultimate Selectivity: Site-Directed ChEmistry and Catalysis at Pt-Sn Alloy Surfaces.....	135
<i>Bruce Koel</i>	
Surface Science Studies of Metal Oxides	136
<i>John M. Vohs</i>	
Gold Atom Release In Surface Oxidation Reactions	137
<i>Cynthia Friend, Xiaoying Liu, Baker Thomas, Weiwei Gao</i>	
Historical Perspectives on ChEmistry and ChEmical Process Development and Innovation at Dow	138
<i>Victor Atiemo-Obeng, Rik Tuinstra, Jack Kruper Jr.</i>	

Ernest W. Thiele: His Impact on ChEmical Engineering	139
<i>Jonathan Worstell</i>	
DuPont: Building on the Past towards a Sustainable Future	140
<i>Ray W. Miller</i>	
Shell Hydroformylation (SHF)	141
<i>Joseph B. Powell</i>	
Past, Present, and Future of Gas to Liquids Technology	142
<i>Sagar B. Gadewar, Daniel J. Auerbach, Eric W. McFarland, Vivek Julka</i>	
The Challenges of Diminishing Natural Capital in the Transition to a Bio-Based Industry	143
<i>Luca Zullo, Deborah Ross</i>	
Water Quality Regulation - the Past 100 Years	144
<i>Steven T. Miano</i>	
Water Quantity Regulation - the Past 100 Years	145
<i>Joseph W. Dellapenna</i>	
Interstate Water Regulation - Historical, Current and Future Direction	146
<i>Kenneth J. Warren</i>	
The Role of Science and Engineering in Water Regulation Over the Past 100 Years	147
<i>James R. May</i>	
A Century of Transport: a Personal Tour	167
<i>Stuart W. Churchill</i>	
A Brief History of the Navier-Stokes Equations: Room for Improvement	196
<i>Howard Brenner</i>	
The Role of Computation in Continuum Transport Phenomena	197
<i>Bruce A. Finlayson</i>	
Biological Applications of Transport Phenomena: Converting Mysteries to Puzzles	223
<i>Edwin N. Lightfoot</i>	
Molecular Simulation as a Foundation for Engineering Models: Impact and Prospects	224
<i>Keith E. Gubbins</i>	
Progress and Outlook for Monte Carlo Simulation	225
<i>Doros N. Theodorou</i>	
Development of Force Fields: From Empiricism to Quantum Mechanics	226
<i>J. Ilja Siepmann</i>	
Accuracy of Simulation Compared to Experimental Measurement	227
<i>Anne M. Chaka</i>	
Building on History: Pathways to Energy Independence and Sustainability through Gasification and Sequestration	228
<i>Judd Swift</i>	
A Century of Petrochemical Advances	235
<i>Bipin V. Vora, Peter R. Pujado</i>	
The Role of Industrial Gases in Fuels & Petrochemicals: Past, Present, and Future	244
<i>Dante Bonaquist</i>	
History of the Development of Lng Technology	254
<i>Chen-Hwa Chiu</i>	
Gasification at a Crossroad	259
<i>Amos Avidan, Lee Schmoe</i>	

Past 100 Years of Refining and Future Expectations	260
<i>Irv Wiehe</i>	
100 Years of Petroleum Refining Catalysts	261
<i>E. Thomas Habib</i>	
A Look at the Advances In Catalysis Over the Past Century and Thoughts on the Challenges for the Future.....	262
<i>Alexis T. Bell</i>	
Turning Surface Science into New Catalysis	263
<i>Mark Barteau</i>	
Selectivity In Surface ChEmistry	264
<i>Andrew J. Gellman</i>	
Selectivity In Ethane Dehydrogenation Over Chromia.....	265
<i>John D. Brooks, David F. Cox</i>	
History of Mixing 1908 to 1940.....	266
<i>Gary K. Patterson</i>	
History of Mixing 1940 to 1965.....	267
<i>Arthur W. Etchells III</i>	
History of Mixing - 1965 to 1985.....	268
<i>Richard V. Calabrese</i>	
History of Mixing 1985 to 1997.....	269
<i>Ronald J. Weetman</i>	
History of Mixing 1997 to 2008.....	270
<i>E. Bruce Nauman</i>	
Future Directions of Mixing Research	288
<i>Richard K. Grenville</i>	
Where Does It Go? a History of Solid Waste Disposal, Flow Control and Recycling.....	289
<i>David G. Mandelbaum, Brendan K. Collins</i>	
Development of Solid Waste Landfills	297
<i>Robert Watts</i>	
The Evolution of Hazardous Waste Law and Regulation	306
<i>Mary Ellen Ternes</i>	
Process Control Education: Past, Present, and Future	307
<i>Thomas F. Edgar</i>	
Predictive Control from Practice to Theory	308
<i>James B. Rawlings</i>	
Predicting the Future of Model Predictive Control	309
<i>Manfred Morari</i>	
On Predicting the Future from the Past in Process Control	310
<i>George Stephanopoulos</i>	
Panel Discussion on the Past, Present, and Future of Process Control.....	311
<i>Thomas F. Edgar, James B. Rawlings, George Stephanopoulos, Manfred Morari</i>	
Progress and Outlook for Molecular Dynamics Simulation	312
<i>Edward J. Maginn</i>	
Molecular Simulation Methods for Transport Properties and Processes	313
<i>Peter T. Cummings</i>	

Progress and Outlook for Mesoscale Simulation	314
<i>Juan J. De Pablo</i>	
Commercial Tools for Molecular Simulation: Current, Intermediate and Long Term Perspectives	315
<i>David Rigby</i>	
Fluid Mechanics and Transport Processes: From Colloid Science to Small Devices.....	316
<i>Howard Stone</i>	
Oriented Assembly of Anisotropic Particles by Capillary Interactions	317
<i>Kathleen J. Stebe, Eric Lewandowski, Jorge A. Bernate, Peter C. Searson</i>	
Randomness and Runniness of Confined Fluids	318
<i>Thomas M. Truskett</i>	
Using Quantitative Modeling of Molecular Transport to Accelerate Development of Membranes for Gas Separations	319
<i>David S. Sholl</i>	
Author Index	