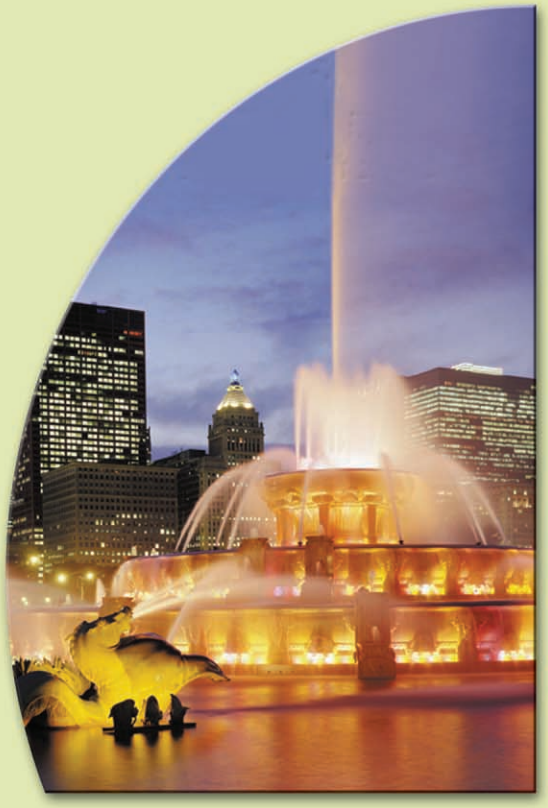
Conference Program Booklet

From Molecular to Product and Process Engineering



ISCRE 18

The 18th International Symposium on Chemical Reaction Engineering

The Palmer House Hilton Hotel
Chicago, Illinois, USA
June 6-9, 2004

Welcome

The Organizing Committee extends a warm welcome to all attendees of the 18th International Symposium on Chemical Reaction Engineering (ISCRE 18). These biennial symposia have a rich history that dates back to 1970, with ISCRE 1 held in Washington, DC. Continuing in the tradition, famous for its architectural beauty, cosmopolitan character, and the splendor of Lake Michigan, Chicago is the host city this year.

The scientific theme for the meeting, "From Molecular to Product and Process Engineering," emphasizes the emerging paradigm that valuable products and novel processes can be engineered based on an understanding of the molecular level interactions. The meeting program includes a broad range of topics, encompassing both traditional and newer fields within the discipline. The goal is to discuss various approaches for the rational application of reaction engineering principles to solve important technological problems facing society.

While participating in the social and technical programs of ISCRE 18, enjoy your stay in Chicago!

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Kurt Vanden Bussche, UOP LLC, ISCRE 18 Co-Chair

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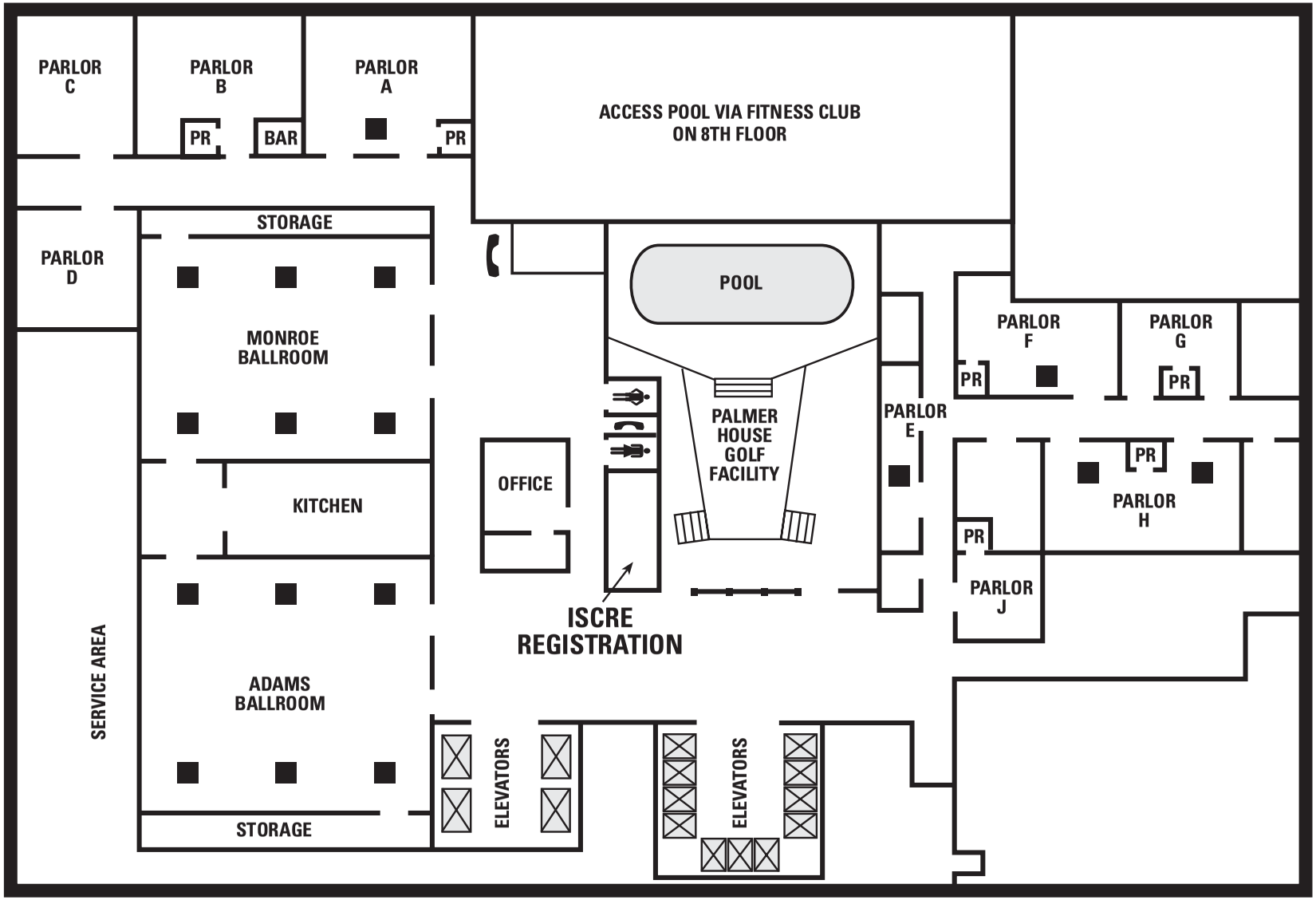

Sixth Floor

CONFERENCE ROOM LOCATIONS ON THE 6TH FLOOR TO THE PALMER HOUSE HILTON

Program at a Glance
Monday, June 7, 2004

Time	Session	Speaker	Location
7:00-8:00 am	Registration		6th floor
8:00-8:10 am	Welcome Remarks	Arvind Varma Bala Subramaniam Kurt VandenBussche	Adams
8:10-9:00 am	Plenary 1	C.N.R. Rao	Adams
9:00-9:50 am	Plenary 2	Wilhelm F. Maier	Adams
9:50-10:20 am	Coffee Break		
10:20 am -12:25 pm	Parallel Oral Sessions 1. Materials Synthesis and Processing 2. Microreaction Technology 3. Catalytic Reactions and Reactors A 4. Computational Fluid Dynamics in Chemical Reaction Engineering A	See Session Details	Parlor H Parlor F Adams Monroe
12:25-2:00 pm	Lunch Break		
2:00-2:50 pm	Plenary 3	Shimshon Gottesfeld	Adams
2:50-3:20 pm	Coffee Break		
3:20-5:25 pm	Parallel Oral Sessions 5. Fuel Cells 6. Polymer Reaction Engineering 7. Environmental Reaction Engineering A 8. Computational Fluid Dynamics in Chemical Reaction Engineering B	See Session Details	Parlor A Parlor F Parlor H Adams
5:30-7:30 pm	Poster Session	See Session Details	Monroe

Program at a Glance
Tuesday, June 8, 2004

Time	Session	Speaker	Location
8:00-8:50 am	Plenary 4	James A. Dumesic	Adams
8:50-9:40 am	Plenary 5	Chaitan Khosla	Adams
9:40-10:10 am	Coffee Break		
10:10 am-12:15 pm	Parallel Oral Sessions 9. Molecular Modeling in Chemical Reaction Engineering A 10. Biological & Biochemical Reaction Eng A 11. Advances in Industrial Processes A 12. Novel Reactors and Processes A	See Session Details	Parlor F Parlor H Monroe Adams
12:15-2:00 pm	Lunch Break		
2:00-2:50 pm	Plenary 6	Sangtae Kim	Adams
2:50-3:20 pm	Coffee Break		
3:20-5:25 pm	Parallel Oral Sessions 13. Molecular Modeling in Chemical Reaction Engineering B 14. Biological & Biochemical Reaction Eng B 15. Multiphase Reactors, Including Pharmaceutical Reactions A 16. Novel Reactors and Processes B	See Session Details	Parlor F Parlor H Monroe Adams
7:00-10:00 pm	Conference Banquet		The Art Institute of Chicago

Program at a Glance
Wednesday, June 9, 2004

Time	Session	Location
8:00-8:50 am	Discussion Forum	Adams
8:50-9:00 am	ISCRE 19 Introduction	Adams
9:00-9:05 am	Transition to Parallel Sessions	
9:05-9:55 am	Parallel Oral Sessions 17. Catalytic Reactions and Reactors B 18. Reactor Dynamics and Control 19. Advances in Industrial Processes B 20. Multiphase Reactors, Including Pharmaceutical Reactions B	 Monroe Parlor F Parlor H Adams
9:55-10:10 am	Coffee Break	
10:10 am-12:15 pm	Parallel Oral Sessions (Continued following Coffee Break) 17. Catalytic Reactions and Reactors B 18. Reactor Dynamics and Control 19. Advances in Industrial Processes B 20. Multiphase Reactors, Including Pharmaceutical Reactions B	 Monroe Parlor F Parlor H Adams
12:15-1:15 pm	Lunch Break	
1:15-2:55 pm	Parallel Oral Sessions 21. Multiphase Reactors, Including Pharmaceutical Reactions C 22. Environmental Reaction Engineering B 23. Novel Reactors and Processes C	 Adams Parlor H Monroe
3:00 pm	Conference Adjourns	

Sunday, June 6, 2004

1:00-5:00 pm	Registration	Palmer House Hilton, 6th floor
5:30-7:00 pm	Opening Reception	The Metropolitan Club (66th floor of the Sears Tower)

Monday, June 7, 2004

7:00-8:00 am Registration [6th floor]

8:00-8:10 am Welcome Remarks [Adams]

A. Varma, ISCRE 18 Chair
B. Subramaniam, ISCRE 18 Co-chair
K. VandenBussche, ISCRE 18 Co-chair

8:10-9:00 am Plenary 1 (Chair: D. Luss) [Adams]

Nanotubes and Nanowires: Synthesis and Properties
C.N.R. Rao
Linus Pauling Research Professor and Honorary President, Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, India

9:00-9:50 am Plenary 2 (Chair: G. Eigenberger) [Adams]

Combinatorial Methods for the Discovery of New Catalysts and Materials
Wilhelm F. Maier
Professor of Chemical Engineering, University of Saarland, Germany

9:50-10:20 am Coffee Break

10:20 am -12:25 pm Parallel Oral Sessions

1. Materials Synthesis and Processing [Parlor H]
2. Microreaction Technology [Parlor F]
3. Catalytic Reactions and Reactors A [Adams]
4. Computational Fluid Dynamics in Chemical Reaction Engineering A [Monroe]

Session 1. Materials Synthesis and Processing

Monday, June 7, 10:20 am -12:25 pm [Parlor H]
Chair: D.W. Hess; Co-Chair: G. Cao

10:20-10:45 Structuring Knowledge on Nanomaterials Processing (invited lecture)
H. Komiyama, University of Tokyo, Japan

10:45-11:10 In-situ Combustion Synthesis of Perovskite Catalysts for Efficient and Clean Methane Pre-mixed Metal Burners
S. Specchia, A. Civera and G. Saracco, Politecnico di Torino, Torino, Italy

11:10-11:35 Microstructural Correlations between Reaction Medium and Combustion Wave Propagation in Heterogeneous Systems
A. Mukasyan, A. Rogachev and A. Varma, University of Notre Dame, IN and Purdue University, West Lafayette, IN

11:35-12:00 Structural Modeling for the Dissolution of Non Porous Ores: Dissolution with Sporulation
A. Adrover, A. Velardo, M. Giona, S. Cerbelli, F. Pagnanelli and L. Toro, Università di Roma, Rome, Italy

12:00-12:25 Nanocasting of Novel, Designer-structured Catalyst Supports
S.P. Rigby, K. Beanlands, M. Watt-Smith and K. J. Edler, University of Bath, Bath, United Kingdom

Session 2. Microreaction Technology

Monday, June 7, 10:20 am-12:25 pm [Parlor F]
Chair: Y. Tonkovitch; Co-Chair: H. Loewe

10:20-10:45 Chemical Micro Process Technology - from Laboratory-scale to Production (invited lecture)
H. Loewe, H. Pennemann and V. Hessel, Institute for Microtechnology, Mainz, Germany

10:45-11:10 Development of a Microstructured Preferential CO Oxidation Reactor and Heat Exchanger Device for a Portable Methanol Fuel Processor
E.R. Delsman, M. de Croon, C. Hofmann, V. Cominos, P. Cobden, G. J. Kramer and J. Schouten, Eindhoven University of Technology, Eindhoven, The Netherlands

11:10-11:35 Heterogeneously Catalysed Oxidation of Carbon Monoxide under Fast Temperature Cycling Conditions
J.J. Brandner, G. Emig, M. A. Liauw and K.Schubert, Forschungszentrum Karlsruhe, Germany

11:35-12:00 Oxidative Dehydrogenation of High Molecular Weight Alcohols in Microreactors
E. Cao, A. Gavriilidis and W.B. Motherwell, University College London, United Kingdom

12:00-12:25 Properties of Free Standing Zeolitic Micromembrane Separator with Different Si/Al ratio.
A.Y.L Yueng, K.L Yeung and M.B. Shing, The Hong Kong University of Science and Technology, Hong Kong, China

Session 3. Catalytic Reactions and Reactors A

Monday, June 7, 10:20 am-12:25 pm [Adams]
Chair: F. Keil; Co-Chair: W. N. Delgass

10:20-10:45 Combinatorial Workflow Development in Heterogeneous Catalysis (invited lecture)
S. Bergh. Symyx Technologies Inc., Santa Clara, CA

10:45-11:10 Real-time in situ FTIR and Raman Analysis of the Liquid Phase Hydrogenation of Maleic Anhydride over Ni-Al/Cu-Zn-Al Catalysts
G.M. Hamminga, G. Mul and J.A. Moulijn, Delft University of Technology, Delft, The Netherlands

11:10-11:35 Development of Spectroscopic Control Methods for Heterogeneously Catalyzed Processes
T.A. Nijhuis, S.J. Tinnemans, T. Visser and B.M. Weckhuysen, Utrecht University, Utrecht, The Netherlands

11:35-12:00 State-by-State Transient Screening of Multi-component Oxide Catalyst in Thin-Zone Multi-Pulse TAP Experiments
S.O. Shekhtman, G.S. Yablonsky, J. T. Gleaves and R.R. Fushimi, Washington University, St. Louis, MO

12:00-12:25 Simultaneous Characterization of Acidic and Basic Properties of Solid Catalysts by a New TPD Method and their Application to Analysis of Reaction Rate
T. Tago, Y. Okubo, T. Tanaka and T. Masuda Hokkaido University, Sapporo, Japan

Session 4. Computational Fluid Dynamics in Chemical Reaction Engineering A

Monday, June 7, 10:20 am-12:25 pm [Monroe]
Chair: R.O. Fox; Co-Chair: B. Andersson

10:20-10:45 Computational Fluid Dynamics for Dense Gas-Solid Fluidized Beds: A Multi-scale Modeling Strategy (invited lecture)
M.A. van der Hoef, M. van Sint Annaland and J.A.M. Kuipers, Twente University, The Netherlands

10:45-11:10 Scale-up of Gas-Phase Chlorination Reactors Using CFD
Y. Liu, V. Raman, R.O. Fox and A.D. Harvey III, Iowa State University, Ames, IA

11:10-11:35 Integrating CFD with Condensation Polymerization Chemistry to Optimize Commercial Multi-jet Pipe Reactors
N.H. Kolhapure, C.J. Pereira and J.N. Tilton, DuPont Engineering Technology, Wilmington, DE

11:35-12:00 Catalyst Design by CFD for Heat Transfer and Reaction in Steam Reforming
M. Nijemeisland, A.G. Dixon and E.H. Stitt, Worcester Polytechnic Institute, Worcester, MA

12:00-12:25 Numerical Simulation of 'Growing' Cu Particles in a Kenics Static Mixer Reactor in which Cu^{++} is Reduced by Carbohydrates
W.F.C. van Wageningen, R.F. Mudde and H.E.A. van den Akker, Kramerslaboratorium, TU-Delft, The Netherlands

12:25-2:00 **Lunch Break**

2:00-2:50 Plenary 3 (Chair: Hyun-Ku Rhee) [Adams]
Direct Methanol Fuel Cells
Shimshon Gottesfeld
Vice President and Chief Technology Officer, MTI Micro Fuel Cells, Albany, NY

2:50-3:20 pm Coffee Break

3:20-5:25 pm Parallel Oral Sessions

5. Fuel Cells [Parlor A]
6. Polymer Reaction Engineering [Parlor F]
7. Environmental Reaction Engineering A [Parlor H]
8. Computational Fluid Dynamics in Chemical Reaction Engineering B [Adams]

Session 5. Fuel Cells

Monday, June 7, 3:20-5:00 pm [Parlor A]
Chair: A. Gavriilidis; Co-Chair: P.J. McGinn

3:20-3:45 High Temperature Polymer Electrolytes for PEM Fuel Cells: Study of the Oxygen Reduction Reaction (ORR) at a Pt –Polymer Electrolyte Interface (invited lecture)
R. Savinell, Case Western Reserve University, Cleveland, OH

3:45-4:10 Combinatorial Processing and Screening of Thin Films for Fuel Cell Electrode Applications
P.J. McGinn, J.S. Cooper and M.A. Black, University of Notre Dame, Notre Dame, IN

4:10-4:35 Physical Model Development, Model Reduction, and Observer Design of a Molten Carbonate Fuel Cell
M. Mangold, M. Sheng, P. Heidebrecht, A. Kienle and K. Sundmacher, Max-Planck-Institut Magdeburg Germany

4:35-5:00 Biomass Reforming Process for Integrated Solid Oxide Fuel Cell Power Generation
S. Vasileiadis and Z. Ziaka-Vasileiadou, ZiVaTech Institute, North Hills, CA

Session 6. Polymer Reaction Engineering

Monday, June 7, 3:20-5:25 pm [Parlor F]
Chair: M. Morbidelli; Co-Chair: B.J. McCoy

3:20-3:45 Analyzing Compositional Drift Transients in Copolymerization Systems using Digital Encoding (invited lecture)
F. Teymour, Illinois Institute of Technology, Chicago, IL.

3:45-4:10 Continuous Precipitation Polymerisation of Vinylidene Fluoride in Supercritical Carbon Dioxide: Modelling the Molecular Weight Distribution
T.S. Ahmed, J. DeSimone and G. Roberts, North Carolina State University, Raleigh, NC and University of North Carolina, Chapel Hill, NC

4:10-4:35 Reaction Characteristic of Decomposition of Solid and High Viscosity Waste Polymers in Supercritical Fluids
M. Sasaki, S. Fujinaga, T. Iwaya, K. Fukuyama, M. Goto and T. Hirose, Kumamoto University, Kumamoto, Japan

4:35-5:00 Polymer Crosslinking Kinetics: Partitioning According to Number of Crosslinks
B.J. McCoy and R. Li, Louisiana State University, Baton Rouge, LA

5:00-5:25 Dynamic Model for Polypropylene Fluidized Bed Reactor: PoRE
Y.M. Harshe, R.P. Utikar and V.V. Ranade, National Chemical Laboratory, Pune, India

Session 7. Environmental Reaction Engineering A

Monday, June 7, 3:20-5:25 pm [Parlor H]
Chair: P–L. Yue; Co-Chair: P. E. Savage

3:20-3:45 Green Reactions in CO_2: Making the Most of CO_2's Useful Properties (invited lecture)
E. J. Beckman, University of Pittsburgh, Pittsburgh, PA

3:45-4:10 Chemistry of CO_2 Mineral Sequestration via pH Swing Process: Kinetic and Mechanistic Studies on the Dissolution of Serpentine and Precipitation of $MgCO_3$
A.-H. Park and L.-S. Fan, Ohio State University, Columbus, OH.

4:10-4:35 Experimental Investigation of Taylor Vortex Photocatalytic Reactor for Water Purification
P.K. Dutta and A.K. Ray, National University of Singapore, Singapore

4:35-5:00 Analysis of Gasification Reaction of Coke Formed using A Miniature Tubing-Bomb Reactor and A Pressurized Drop Tube Furnace under High Pressure and High Temperature
K. Miura, H. Nakagawa, S. Nakai and S. Kajitani, Kyoto University. Kyoto, Japan

5:00-5:25 Photo-Doping Technique as a Novel Preparation Method for the Photo-Fenton Catalyst and its Potential Application for Wastewater Treatment
F. L. Y. Lam, J.U.C. Fong and X. Hu, Hong Kong University of Science and Technology, Hong Kong, China

Session 8. Computational Fluid Dynamics in Chemical Reaction Engineering B

Monday, June 7, 3:20-5:25 pm [Adams]
Chair: H. Kuipers; Co-Chair: E.H. Stitt

3:20-3:45 Three Dimensional Simulation of Bubble Columns Flows: Influence of Bubble Coalescence and Breakup
P. Chen, J. Sanyal and M.P. Dudukovic, Washington University, St. Louis, MO

3:45-4:10 Momentum and Mass Transfer in a Swarm of Bubbles: Estimates from Fluid-Dynamic Simulations
F. Bertola, G. Baldi, D. Marchisio and M. Vanni, Politecnico di Torino, Italy

4:10-4:35 A Three-Dimensional Simulation of Gas/Particle Flow and Ozone Decomposition in the Riser of a Circulating Fluidized Bed
J K.G. Hansen, T. Solberg and B.H. Hjertager, Aalborg University Esbjerg, Denmark

4:35-5:00 Modeling and Simulation of a Catalytic Gas-Solid Fluidized Bed Reactor via DEM
S. Limtrakul, A. Boonsirat, Y. Tsuji, T. Kawaguchi and T. Tanaka, Kasetsart University, Thailand

5:00-5:25 CFD Modeling of Chemical Reactors: Homogeneous and Heterogeneous Reaction
L. Rudniak, P. M. Machniewski, A. Milewska and E. Molga, Warsaw University of Technology, Poland

Poster Session

Monday, June 7, 5:30-7:30 pm [Monroe]

Topic 01. Molecular Modeling in Cemical Reaction Engineering

1. Statistical Mechanical Treatment of Hydrocarbon Adsorption on Zeolites: Adsorption on Silicalite of Benzene and Alkane Binary Mixtures
   S.E. Jalili, G. Manos and L.J. Dunne, University College London, London, United Kingdom

2. Reaction Route Graphs as a Tool for Microkinetic Modeling and Reduction: Application to the Water-Gas-Shift Reaction
   Q. Callaghan, I. Fishtik and R. Datta. Worcester Polytechnic Institute, Worcester, MA

3. N-paraffins Hydrocracking Model
   L. Pellegrini, V. Calemma, S. Locatelli and S. Rasella. Politecnico of Milan, Italy

4. Modeling 'Molecular Square' Catalysts: A Multiscale Approach
   D. Majumder, M. Curet-Arana, R.Q. Snurr and L.J. Broadbelt. Northwestern University, Evanston, IL

5. Chemical System Identification in Liquid Phase Transition-Metal Homogeneous Catalysis
   W. Chew, C. Li, E. Widjaja and M.Garland. National University of Singapore, Singapore

6. Study of 4,6-bis(nitroamino)-1,3,5-triazin-2(1\emph{H})-one, Related Tautomers and Conformers
   P. Simoes, L. Pedroso and A. Portugal. Universidade de Coimbra - Faculdade de Ciencias e Tecnologia, Coimbra, Portugal

7. Microkinetic Modeling of Light Paraffin Aromatization on ZSM-5 based Catalysts
   A. Bhan, S.H. Hsu, C.K. Tn, V. Venkatasubramaniam, D. Thomson, J. Caruthers and W.N. Delgass. Purdue University, West Lafayette, IN

8. Molecular Modeling of Water-gas Shift and Preferential Oxidation of CO Reactions
   D. Vlachos and A. B. Mhadeshwar. Univ. of Delaware, Newark, De

9. Rule-Based Refinement and Feature Matching in Kinetic Modeling
   S.-H. Hsu, A. Bhan, W. N.Delgass, J.M. Caruthers and V. Venkatasubramanian, Purdue University, West Lafayette, IN

Topic 02. Microreaction Technology

10. Microchannel Process Technology (MPT)™ for Compact Methane Steam Reforming
    A.Y. Tonkovich, Y. Wang, Steve Perry, D. Qiu and W. A. Rogers. Velocys, Inc., Plain City, OH

11. Study on the Hydrodynamics and Gas Mixing of Carbon Nanotubes (CNTs) in a Nano-agglomerates Fluidized Bed (NAFBR)
    Y. Hao, W. Fei, W. Yao and L. GuoHua, Tsinghua University, Beijing, China

12. Compositional and Structural Optimal Design of a Nanostructured Diesel-soot Combustion Catalyst for a Fast-regenerating Catalytic Trap
    D. Fino and V. Specchia, Politecnico di Torino, Italy

Topic 03. High Throughput Synthesis and Screening

13. Combinatorial Chemistry for Heterogeneous Catalysis: Parallel Reactor Systems for Flexible Screening and Optimization
    D. Akporiaye, J. Bennetsen, A. Karlsson, M. Plassen, E. Myhrvold, M. Bricker, R. Gillespie, C. McGonegal and A. Sachtler, Torial, Des Plaines, IL

Topic 04. Fuel Cells

14. Study on CO_2 Reforming of Methane to Syngas over Al_2O_3-ZrO_2 Supported Ni Catalysts Prepared via a Direct Sol-gel Processing
    H. Li and J. Wang, Tsinghua University, Beijing, China

15. Nonlinear Analysis of Current Instabilities in High Temperature Fuel Cells
    M. Mangold, M. Krasnil and K.Sundmacher, Max-Planck-Institut Magdeburg, Germany

16. Integrated Concepts for the Decentralized Production of Clean Hydrogen
    A. Gritsch, B. Gloeckler, E. Lopez; A. Morillo and G. Eigenberger. Institute for Chemical Process Engineering, University of Stuttgart, Germany

Topic 05. Novel Reactors and Processes

17. Hydrodynamics and Mass Transfer in an Upflow Monolith Loop Reactor
    C.O. Vandu, J. Ellenberger and R. Krishna, University of Amsterdam, The Netherlands

18. Radiative Transfer within a Fluidized Bed Reactor for Steam-gasification of Coal
    P. Van Zedtwitz and A. Steinfelds, ETH - Swiss Federal Institute of Technology, Zurich, Switzerland

19. Reaction Calorimetry in Supercritical Carbon Dioxide
    F. Lavanchi, S. Fortini and Th. Meyer, Swiss Federal Institute of Technology, Lausanne, Switzerland

20. Pulsed Compression Reactor: Advanced Technology for Synthesis Gas Production
    M. Glouchenkov and A. Kronberg, University of Twente, Enschede, The Netherlands

21. Microwave Dielectric Heating as a Gateway to Process Intensification.
    J.P. Mikkola, B.Toukoniitty, K. Eranen and T. Salmi, Åbo Akademi University, Turku, Finland

22. Application of Film-Flow-Monoliths and Structured Packings in Reactive Stripping.
    T.J. Schildhauer and F. Kapteijn, Technical University Delft, The Netherlands

23. Direct Synthesis of Oxygenates from Water Vapor and Methane via Glow Discharge with Rotating Ploy-tip Electrodes.
    B.W. Wang and G.H. Xu, Tianjin University, Tianjin, China

24. Pattern-enhanced Micro-fluidized Bed Reactor.
    J. Li, I.S. Aranson and W.K. Kwok, Argonne National Lab, Argonne IL

25. Process Intensification, Characterization, and Control of Reactive Systems
    L.F.S. Mascolo, M.H.M. Reis, J.F. Pinto and M.R.Wolf-Maciel, Universidade Estadual de Campinas, Brazil

26. Gas-Liquid-Solid Catalytic Hydrogenation Reaction in a Single Monolith Channel
    W. Liu and S. Roy, Corning Incorporated, Corning, NY

27. Analysis of Tubular Packed-bed Membrane Reactors Based on Nonisothermal 2D-reactor models
    A. Tota, C. Hamel, E. Tsotsas and A. Seidel-Morgenstern, Otto von Guericke University Magdeburg Germany

28. Light Intensity Distribution in Photocatalytic Reactors: Effect of Catalyst Loading and Wall Reflectivity
    V.K. Pareek and A.A. Adesina, Curtin University of Technology Perth, Australia

29. Hydrodynamics of a Novel Monolithic Stirrer Reactor: Experiments and Numerical Simulations
    H.P. Kritzinger, C.R. Kleijn and H.E.A. Van den Akker, Delft University of Technology, Delft, The Netherlands

30. Towards More Effective Reactor Configurations for FTS: Issues of Selectivity, Catalyst Life and Safety
    Q. Qin, D. Ramkrishnaa and R.Espinoza, Purdue University, West Lafayette, IN

Topic 06. Novel Biological and Biochemical Reaction Engineering

31. Simulation of Biodegradation of Synthetic Wastewater at Higher Concentrations in a Fluidized-bed Bioreactor with an Internal Draft Tube
    A. Venu Vinod and V.R. Goli, National Institute of Technology, Warangal, India

32. Design of SSF Bioreactor for Food Enzymes Production.
    R. Ravinder, P. Ravindra and B. Rao, Osmania University, Hyderabad, India

33. Enrichment of n-3 PUFA Contents in GIcerides of Fish Oil by Lipase-Catalyzed Ester Interchange under Supercritical Conditions
    T.-J. Lin, S.-W. Chen and A.-C. Chung, National Chung-Cheng University, Chia-Yi, Taiwan R.O.C.

34. Models for Macromolecular Folding and Denaturation Based on Kinetics of Energy Landscapes
    B.J. McCoy and J. Yang, Louisiana State University, Baton Rouge, LA

35. Oxygen Transfer Effects on Recombinant Benzaldehyde Lyase Production
    P. Calik, P. Yilgor, P. Ayhan and A.S. Demir, Middle East Technical University, Ankara, Turkey

36. Carbon Sources Create Fingerprint Fermentation Characteristics: Serine Alkaline Protease Production.
    T. Ozdamar and G. Calik, Ankara University, Ankara, Turkey

37. Modeling and Design of Biodegradable Polymeric Microspheres for Controlled Drugs Delivery
J. Pan, Y. Qian, L. Zhang and Y. Jiang, South China University of Technology, Guangzhou, China

38. Determinants of Pulmonary Oxygen Uptake: A Novel Multi-scale Engineering Approach.
S. Chakraborty, A. Bidani and V. Balakotaiah, University of Houston, Texas

Topic 07. Materials Synthesis and Processing

39. Controlling the Micromorphologies of Porous Silica Gels Synthesized by Unidirectional Freeze-gelation.
S.R. Mukai, H.Nishihara and H.Tamon, Kyoto University, Kyoto, Japan

40. Chemical Vapor Deposition Rate of Pyrolytic Carbon from Hydrocarbons.
M. Kawase, T. Nakai, H. Goshima and K. Miura, Kyoto University, Kyoto, Japan

41. Preparation of Monolithic Silica-Titania Aerogels by Modified Sol-Gel Method
S. Cao, K.L. Yeung and P.-L. Yue, The Hong Kong University of Science and Technology, Hong Kong, China

42. Advanced Modeling of Self-propagating High Temperature Synthesis.
A.M. Locci, A. Cincotti, F. Delogu, R. Orru and G. Cao, University of Cagliari, Italy

43. Production of Carbon Nanotubes of Controlled Structure and Development of Nanotube-based Materials
D. Resasco, J. E. Herrera, L. Balzano and O. Matarredona, University of Oklahoma, Norman, OK

Topic 08. Polymer Reaction Engineering

44. Property Control in a Continuous Polymerization Reactor using Wiener Model Predictive Controller with One Step Identification
I.-H. Song and H.-K. Rhee, Seoul National University, Seoul, Republic of Korea

45. Estimation of Intrinsic Rate Coefficients in Vinyl Chloride Suspension Polymerization
T. De Roo, G.J. Heynderickx and G.B. Marin, Ghent University, Ghent, Belgium

46. Morphogenesis of Polyolefin Particles in Heterogeneous Catalytic Reactors: Effect of Temperature
J.Kosek, Z. Grof and M.Marek, Prague Institute of Chemical Technology, Prague, Czech Republic

47. Kinetic Rate of Emulsion Copolymerization of Styrene and Natural Rubber Latex
T. Vatanatham and C. Meepetchtan, Kasetsart University, Bangkok, Thailand

Topic 09. Computational Fluid Dynamics in Chemical Reaction Engineering

48. Optimization of Gas – Liquid Reactor Using Computational Fluid Dynamics
A.W. Patwardhan, J.B. Joshi, S. Fotedar and T. Mathew, Institute of Chemical Technology, Mumbai, India

49. A Novel Coupled Riser-Downer Reactor: Industrial Trial and CFD Simulation of Reacting Flows
F. Liu, Y. Cheng and F. Wei, Tsinghua University, Beijing, China

50. A Numerical Approach to Study Transport Limited Heterogeneous Reactions
K. Deshpande and W.B. Zimmerman, University of Sheffield, United Kingdom

51. CFD Simulations to Study Early Shortstop of Runaway Reaction in Stirred Vessel
D. Dakshinamoorthy, A.R. Khopkar, J.F. Louvar and V.V. Ranade, National Chemical Laboratory, Pune, India

52. Influence of the Turbulence Model in CFD Modeling of Wall to Fluid Heat Transfer in Packed Beds
A. Guardo, M. Coussirat, M.A. Larrayoz, F. Recasens and E. Egusquiza, Universitat Politecnica de Catalunya, Barcelona, Spain

53. Micro Combustion for Localized Heat Generation/Delivery
M. Sangalli, K.M. VandenBussche, G.P. Towler and A.R. Oroskar, UOP LLC, Des Plaines, IL

Topic 10. Environmental Reaction Engineering

54. Rapid Oxidation of Sulfide Mine Tailings by Reaction with Potassium Ferrate
D.A. Rockstraw, M. Murshed, A.T. Hanson and M. Johnson, New Mexico State University, Las Cruces, NM

55. Decomposition and Oxidation of Aliphatic Nitro Compounds in Supercritical Water: Kinetics and Effect of Pressure
V. Anikeev, A. Yermakova and M. Goto, Institute of catalysis, Novosibirsk, Russia

56. Catalytic Wet Air Oxidation of Phenol over Active Carbon: Trickle Bed Kinetics and Reactor Modelling
A. Eftaxias, J. Font, A. Fortuny, A. Fabregat and Frank Stueber, Universitat Rovira i Virgili, Tarragona, Spain

57. Modeling of Urea-SCR Process to Remove NO from Diesel Engine over CuZSM5 Catalyst
J.H. Baik, S.D. Yim, I.-S. Nam, Y.S. Mok, J.-H. Lee, B.K. Cho and S. H. Oh, Pohang University of Science & Technology (POSTECH), Pohang, Republic of Korea

58. SCR-DeNO_x for Diesel Exhaust After-treatment: Unsteady-state Kinetic Study and Monolith Reactor Modeling
C. Ciardelli, I. Nova, E. Tronconi, B. Konrad, D. Chatterjee, K.Ecke and M. Weibel, Politecnico di Milano, Italy

59. Ignition Enhancement by In Situ Generated C_2 Additives for Natural Gas Practical Combustion Applications
J.A. Langille, J. Pasale, F.N. Egolfopoulos and T.T. Tsotsis, University of Southern California, Los Angeles, CA

60. Photo Absorption and Forward Scattering in TiO_2 Photocatalytic Slurry Reactors
M. Salaices, B. Serrano and H. de Lasa, University of Western Ontario, London, Canada

61. Destruction of Cationic Ion-exchange Resin in a Molten Salt Oxidation Reactor.
H.C. Yang, Y.-J. Cho, H.-C.Eun, J.-H. Yoo and J.-H. Kim, Korea Atomic Energy Research Institute. Daejon, Republic of Korea

62. Dynamics of Storage and Reaction in a Monolith Reactor: Lean NO_x Reduction
K. Kabin, R. Muncrief and M. Harold, University of Houston, Texas

63. Reactor Design Issues for Enhancing High Voltage Electrical Discharge Reactors to Degrade Aqueous Phase Contaminants
M. Sahni, D. Tondeur and M.A. Latifi, Florida State University, Tallahassee, FL

64. Explaining Inhibition and Acceleration of Phenol SCWO by Water
J.H. Henrikson and P.E. Savage, University of Michigan - Ann Arbor, MI

65. A Multifunctional Filter for the Simultaneous Removal of Fly-ashes and Nox from Incinerator Flue Gases
    G. Saracco, D. Fino, N. Russo and V. Specchia, Politecnico di Torino, Italy

Topic 11. Multiphase Reactors, including Pharmaceutical Reactions

66. Estimation of Trickle-to-pulse Flow Regime Transition and Pressure Drop in High-pressure Trickle Bed Reactors with Organic Liquids.
    M.I. Urseanu, J.G. Boelhouwer, H.J.M. Bosman, J.C. Schroijen and G. Kwant, DSM Research, Geleen, The Netherlands

67. Mathematical Modeling of Multifunctional Reactor for Direct Conversion of Methane to Methanol.
    V. Kafarov and C. Dallos, Universidad Industrial de Santander, Bucaramanga, Colombia

68. Benzene Nitration: Validation of Heterogeneous Reaction Models
    P.A. Quadros, N.M.C. Oliveira and C.M.S.G. Baptista, Department of Chemical Engineering, University of Coimbra, Portugal

69. Holdups and Pressure Drop in Multiphase Monolithic Reactors
    T. Bauer, S. Roy, M. Al-Dahhan and R. Lange, Dresden University of Technology, Dresden, Germany

70. Dynamic 2D Simulation of the Startup Processes in Circular Two-phase Bubble Columns
    H. Lindborg, C.A. Dorao, F. Bertola and H.A. Jakobsen, Norwegian University of Science and Technology, Trondheim, Norway

71. Scale-up of Gas-Liquid Monolith Reactors
    M.T. Kreutzer, J. Bakker and J.A. Moulijn, Delft University of Technology, Delft, The Netherlands

72. Mass Transfer and Fluid Dynamic Effects on Kinetic Studies in Small Scale G-L Upflow Hydrotreaters
    G.B. Bellos, K.P. Gotsis, P.A. Galtier and N.G. Papayannakos, National Technical University of Athens, Athens, Greece

73. Liquid Phase Oxidations in Multichannel Reactor
    P.K. Plucinski and A.A. Lapkin, University of Bath, United Kingdom

74. Simulation and Experiment Study of Dimethyl Ether Synthesis from Syngas in a Fluidized-Bed Reactor
    W.Z. Lu, L.-H. Teng and W.-D. Xiao, East China University of Science and Technology, Shanghai, China

75. Reaction Kinetics Accompanied by Partial Internal Wetting of Catalysts under Elevated Temperature and Pressure
    Z.M. Zhou, Z. Cheng and Z. Li, East China University of Science and Technology, Shanghai, China

76. A Numerical Study on Coalescence and Breakage in Bubble Column Reactors
    S. Bove, T. Solberg and B.H. Hjertager, Aalborg University, Esbjerg, Denmark

77. Analysis of Heterogeneously Catalyzed Fast Gas-Liquid Reactions
    J.A. Raffensberger, B.Glasser and J.Khinast, Rutgers University, Piscataway, NJ

78. An Analysis of Particle-liquid Slip Velocities in Multiphase Stirred Tank Reactors using Positron Emission Particle Tracking.
R.P. Fishwick, J.M. Winterbottom, D.J. Parker and X. Fan, University of Birmingham, United Kingdom

Topic 12. Catalytic Reactions and Reactors

79. Control of Acid Site Distribution of MFI-type Zeolite by Selective Formation of SiO_2 Unit Utilizing Silane Compounds with Different Molecular Sizes
T. Tago, K. Tanaka K. Morita T. Tsuji and Takao Masuda, Hokkaido University, Sapporo, Japan

80. Modeling the Effect of Catalyst Particle Lyophobicity on Mass Transfer and Reaction Rate at the Gas-liquid Interface in a Gas Inducing Stirred Slurry Reactor
K.C. Ruthiya, J. van der Schaaf, B.F.M. Kuster and J.C. Schouten, Eindhoven University of Technology, Eindhoven, The Netherlands

81. Kinetics and Trickle-bed Reactor Model for Direct Synthesis of Hydrogen Peroxide
L. Li, K.M. VandenBussche, M.Sangalli and G.P.Towler, UOP LLC, Des Plaines, IL

82. Effective Carbon Dioxide Fixation from Epoxides to Cyclic Carbonate by using Supercritical CO_2-ionic Liquid Reaction System
H. Kawanami and Y. Ikushima, National Institute of Advanced Industrial Science and Technology, Sendai, Japan

83. The Temperature Scanning Plug Flow Reactor (TSPFR) Applied to Complex Reactions — Oxidative Dehydrogenation of Propane as an Example
M. Kolkowski, F.J. Keil, C. Liebner, D. Wolf and M. Baerns, Hamburg University of Technology, Hamburg, Germany

84. The Site-Juxtaposition Model of Catalyst Deactivation: Simulation and Experiments During *n*-pentane Isomerization on a Highly Active and Stable Pt-sulfated Zirconia Catalyst.
S. Vijay and E.E. Wolf, University of Notre Dame, Notre Dame, IN

85. A New Technique for Studying the Internal Physical Structure of a Supported Catalyst or Sorbent Particle
P. Gupta and L.-S. Fan, The Ohio State University, Columbus, OH

Topic 13. Reactor Dynamics and Control

86. Multiscale Systems Engineering with Applications to Chemical Reaction Processes
R.D. Braatz, R.C. Alkire, E.G. Seebauer, T.O. Drews, R. Gunawan, M.Y. L. Jung and E. Rusli, Univeristy of Illinois at Urbana-Champaign, IL

87. Investigation of Hybrid N2O-decomposition in Structured Catalyst Beds under Periodical Operating Conditions
F. Platte and K. Nalpantidis, University of Dortmund, Department of Biochemical and Chemical Engineering, Dortmund, Germany

88. Optimal Design, Operation and Control of Different Variants of a Simulated Moving Bed Reactor
A.S. Karup, Y. Zhang, K. Hidajat and A.K. Ray, National University of Singapore, Singapore

89. Modeling Temporally-complex Breathing Patterns during Pd-Catalyzed CO Oxidation
    M. Sheintuch, O. Nekhamkina and R. Digilov, Technion, Haifa, Israel

90. Steady State and Dynamic Reactor Models for Coupling Exothermic and Endothermic Reactions.
    R.C. Ramaswany, P.A. Ramachandran and M.P. Dudukovic, Washington University, St Louis, MO

91. Real-time Estimation and Feedback Control of Surface Roughness of PECVD Amorphous ZrO_2 Thin Film Growth
    D. Ni, Y. Lou and P. D. Christofides, University of California, Los Angeles, CA

92. A Systematic Approach for Analyzing Regenerative Multifunctional Reactors
    G. Kolios, R. Garg and D. Luss, ICVT, University of Stuttgart, Germany

Topic 14. Advances in Industrial Processes

93. Mathematical Modeling of Liquid-phase Decomposition through Gas-phase Product Analysis
    N. Musakka, T. Salmi, J. Warna, J. Ahlkvist and M. Piironen, Åbo Akademi University, Turku, Finland

94. A Model for the Oxidation of Toluene under Industrial Conditions
    J.A.A. Hoorn, M. Hoorneman and G.F. Versteeg, DSM Research, Geleen, The Netherlands

95. Engineering Aspects of Manufacturing Tri-*n*-Butyl Phosphate Esters
    S. Waje, A.S. Gudekar, B.N. Thorat and A.U. Mehta. University Institute of Chemical Technology (UICT), Mumbai, India

96. The Effect of Additives on Industrial Precipitation of a Di-substituted Benzoic Acid
    P.A. Oinas and R. Davey, Kemira Fine Chemicals Oy, Kokkola, Finland

Tuesday, June 8, 2004

8:00-8:50 am Plenary 4 (Chair: T. R. Keane) [Adams]

Molecular modeling and Microkinetics for Rational Design of Processes
James A. Dumesic
Steenbock Professor of Chemical Engineering, University of Wisconsin

8:50-9:40 am Plenary 5 (Chair: L. L. Hegedus) [Adams]

Biosynthesis of Pharmaceutical Products
Chaitan Khosla
Professor of Chemical Engineering, Chemistry and Biochemistry (by courtesy), Stanford University

9:40-10:10 am Coffee Break

10:10 am-12:15 pm Parallel Oral Sessions

9. Molecular Modeling in Chemical Reaction Engineering A [Parlor F]
10. Biological & Biochemical Reaction Eng A [Parlor H]
11. Advances in Industrial Processes A [Monroe]
12. Novel Reactors and Processes A [Adams]

Session 9. Molecular Modeling in Chemical Reaction Engineering A

Tuesday, June 8, 10:10 am-12:15 pm [Parlor F]
Chair: C.R. Kennedy; Co-Chair: M.O. Coppens

10:10-10:35 Computational Catalysis Towards the Elucidation and Design of Active Catalytic Environments (invited lecture)
M. Neurock, S.A. Wasileski and D. Mei, School of Engineering and Applied Science, Charlottesville, VA

10:35-11:00 A Monte Carlo Study of the Selective Hydrogenation of Acetylene
A. McLeod, Imperial College London, United Kingdom

11:00-11:25 Non-isothermal Dynamic Monte Carlo Simulations of CO Oxidation on Pt Supported Catalysts
F.J. Gracia and E.E. Wolf, University of Notre Dame, Notre Dame, IN

11:25-11:50 A Mechanistic Simulation Model for NOx Storage Catalyst Dynamics
U. Tuttlies, V. Schmeisser and G. Eigenberger, ICVT, Stuttgart, Germany

11:50-12:15 Analysis of a Carbon Membrane Reactor: from Atomistic Simulations of Single File Diffusion to Reactor Design.
M. Sheintuch and G. Sznejer, Technion, Haifa, Israel

Session 10. Biological & Biochemical Reaction Engineering A

Tuesday, June 8, 10:10 am-12:15 pm [Parlor H]
Chair: D. Ramkrishna; Co-Chair: S. Sicardi

10:10-10:35 Metabolic Engineering: Extending the Paradigm of Reaction Engineering to the Analysis and Design of Bioreaction Pathways (invited lecture)
G. Stephanopoulos, Massachusetts Institute of Technology, Cambridge, MA

10:35-11:00 Metabolic Engineering of Aromatic Group Amino Acid Pathway in Bacillus Subtilis for L-Phenylalanine Production
I. Senver-Ozcelik and T.H. Ozdamar, Ankara University, Turkey

11:00-11:25 Enzymatic Synthesis of Biotensides from Renewable Sources
E.M. del Amor Villa and R. Wichmann, University of Dortmund, Germany

11:25-11:50 Structured Reactors for Enzyme Immobilization
K. A. de Lathouder, J. Bakker; F. Kapteijn and S.A. Wallin, Dow Chemical Company, Midland, MI

11:50-12:15 Modeling of Engineered Cartilage Growth in Rotating Bioreactors
M. Pisu, N. Lai, A. Cincotti and G. Cao, University of Cagliari, Italy

Session 11. Advances in Industrial Processes A

Tuesday, June 8, 10:10 am-12:15 pm [Monroe]
Chair: S.B. Jaffe; Co-Chair: H. de Lasa

10:10-10:35 Metabolic Engineering for the Microbial Production of 1,3-Propanediol (invited lecture)
A.W.Alsop, DuPont CR&D, Wilmington, DE

10:35-11:00 Monolith Reactors: Scale-up and Process Intensification
T. Haakana, L. Ronkko, I. Turunen, J.-P. Mikkola, J. Warna, J. Aumo and T. Salmi,
Lappeenranta University of Technology, Finland

11:00-11:25 Ebullated Bed Reactor Modeling for Residue Conversion
J.M.S Schweitzer and S. Kressman, Institut Francais du Petrole, France

11:25-11:50 Computational Fluid Dynamic Analysis of HVOF Thermal Spray Processing of Nanostructured Coatings
M. Li, D. Shi and P.D. Christofides, University of California, Los Angeles, CA

11:50-12:15 High-Emissivity Coatings on Reactor Tubes and Furnace Walls in Pyrolysis Furnaces
G.J. Heynderickx and M. Nozawa, Ghent University, Belgium

Session 12. Novel Reactors and Processes A

Tuesday, June 8, 10:10 am-12:15 pm [Adams]
Chair: T.T. Tsotsis; Co-Chair: E. J. Beckman

10:10-10:35 The Use of Zeolite Films in Microscale Applications (invited lecture)
J. Santamaria, University of Zaragoza, Zaragoza, Spain

10:35-11:00 Catalytic Hydroformylation of 1-octene in CO_2-Expanded Solvent Media
H. Jin and B. Subramaniam, University of Kansas, Lawrence, KS

11:00-11:25 One Step Production of Fine Chemicals using Supercritical Water: An Environmentally Benign Application to the Synthesis of Mono-terpene Alcohol.
Y. Ikushima, M. Sato and K. Hatakeda, National Institute of Advanced Industrial Science & Technology, Sendai, Japan

11:25-11:50 Acid- and Base-catalyzed Organic Synthesis in High-temperature Liquid Water
S.E. Hunter and P.E. Savage, University of Michigan, Ann Arbor, MI

11:50-12:15 Development of a Multi-scale Simulation Method for Design of Novel Multiphase Reactors
R. Andersson, B. Andersson, F.Chopard and T. Noren, Chalmers University of Technology, Gothenburg, Sweden

12:15-2:00 pm **Lunch Break**

2:00-2:50 pm Plenary 6 (Chair: V .W. Weekman) [Adams]

Informatics and Reaction Engineering for Pharmaceutical R&D
Sangtae Kim
Feddersen Distinguished Professor of Mechanical Engineering and Chemical Engineering, Purdue University

2:50-3:20 pm Coffee Break

3:20-5:25 pm Parallel Oral Sessions

13. Molecular Modeling in Chemical Reaction Engineering B [Parlor F]
14. Biological & Biochemical Reaction Eng B [Parlor H]
15. Multiphase Reactors, Including Pharmaceutical Reactions A [Monroe]
16. Novel Reactors and Processes B [Adams]

Session 13. Molecular Modeling in Chemical Reaction Engineering B

Tuesday, June 8, 3:20-5:00 pm [Parlor F]
Chair: M. Neurock; Co-Chair: M. Sheintuch

3:20-3:45 Dynamic Monte Carlo Simulations of Multi-component Diffusion in Zeolites: Effect of Strong Adsorption Sites
V.R. Iyengar and M.-O. Coppens, Delft University of Technology, Delft, The Netherlands

3:45-4:10 Molecular Reconstruction of LCO Gasoils from Overall Petroleum Analyses
D. Hudebine and J.J. Verstraete, Institut Francais du Petrole, Vernaison, France

4:10-4:35 Relumped Single Event Microkinetic Model for Alkane Hydrocracking on Shape Selective Catalysts: Catalysis on ZSM-22 Pore Mouths, Bridge Acid Sites and Micropores
C.S. Narasimhan, J.W. Thybaut, G.B. Marin, J. F. Denayer, G.V. Baron, J.A. Martens and P.A. Jacobs, Ghent University, Ghent and Leuven University, Leuven, Belgium

4:35-5:00 A Single Events Kinetic Model: n-butane Isomerization
K. Surla, H. Vleeming, D. Guillaume and P. Galtier, Institut Francais du Petrole, Vernaison, France

Session 14. Biological & Biochemical Reaction Engineering B

Tuesday, June 8, 3:20-5:25 pm [Parlor H]
Chair: G. Stephanopoulos; Co-Chair: A. W. Alsop

3:20-3:45 Cybernetic Modeling of Metabolism: Towards a Framework for Rational Design of Recombinant Organisms
J.D. Young, K. Henne, J.A. Morgan, A.E. Konopka and D. Ramkrishna, Purdue University, West Lafayette, IN

3:45-4:10 Computational Framework for the Discovery of Novel Biotransformations
L. Broadbelt, V. Hatzimanikatis, C. Li, M. Jankowski, C. Henry, J. Gonzalez and J. Ionita, Northwestern University, Evanston, IL

4:10-4:35 Hybrid Neural-Networks Modeling of an Enzymatic Membrane Reactor
M. Al-Yemni and R.Y.K. Yang, SABIC R&T

4:35-5:00 Modeling of Enzymatic Membrane Reactor for the Resolution of Racemic Ibuprofen Ester
S. Bhatia, A. H. Kamaruddin and W. Sing Long, University Science of Malaysia

5:00-5:25 Effect of Biochemical Reactions in Enhancement of Rate of Leaching
D.R. Ravindra and B. Kodali, Osmania University, India

Session 15. Multiphase Reactors, Including Pharmaceutical Reactions A

Tuesday, June 8, 3:20-5:25 pm [Monroe]
Chair: M. P. Dudukovic; Co-Chair: J. Schouten

3:20-3:45 Multiphase Catalysis and Reaction Engineering for Emerging Pharmaceutical Processes (invited lecture)
R.V. Chaudhari, NCL Pune, India

3:45-4:10 FastCat Reactor for HTS of Gas-Solid Catalyzed Reactions
P.L. Mills and J.F. Nicole, DuPont Company, Wilmington, DE

4:10-4:35 Unsteady-State Operation of Trickle-Bed Reactors
R. Lange, M. Schubert, W. Dietrich and M. Gruenewald, Dresden University of Technology, Dresden, Germany

4:35-5:00 Performance of Catalytic Membrane Reactor in Multiphase Reactions
M. Vospernik, A. Pintar, G. Bercic and J. Levec, National Institute of Chemistry, Ljubljana, Slovenia

5:00-5:25 Packings for Fixed Bed Reactors and Reactive Distillation
C. Miller and G. Kaibel, BASF AG, Ludwigshafen, Germany

Session 16. Novel Reactors and Processes B

Tuesday, June 8, 3:20-5:25 pm [Adams]
Chair: J.J. Lerou; Co-Chair: J. Santamaria

3:20-3:45 Loop Reactor Staged with Structured Catalytic Layers for Liquid-Phase Hydrogenation
L. Kiwi-Minsker, E. Joannet and A. Renken, Swiss Federal Institute of Technology, Lausanne, Switzerland

3:45-4:10 Effect of Monolith Catalyst Channel Shape on Gas-Liquid Catalytic Performance
W. Liu and S. Roy, Corning Inc., Corning, NY

4:10-4:35 Monolithic Catalysts with 'High Conductivity' Honeycomb Supports for Gas/solid Exothermic Reactions: Characterization of the Heat-transfer Properties
E. Tronconi, G. Groppi, T. Boger and A. Heibel, Politecnico di Milano, Milano, Italy, and Corning Inc., Corning, NY.

4:35-5:00 Design of Stationary Phase Properties for Optimal Performance of Reactive of Reactive Simulated-Moving-bed Chromatography
G. Stroehlein, M. Mazzotti and M. Morbidelli, ETH, Zürich, Switzerland

5:00-5:25 Nanoporous Silicon Carbide Membranes, Preparation and Reactive Applications.
B.F.N. Fayyaz, K. Molaaie-Nezhad, H. Patel, R.J. Ciora, P.K.T. Liu, M. Sahimi and T.T. Tsotsis,
University of Southern California, Los Angeles, CA

7:00-10:00 pm **Conference Banquet** **[The Art Institute of Chicago]**

Wednesday, June 9, 2004

8:00-8:50 am Discussion Forum (Chair: A. Varma) [Adams]

Future Directions in Chemical Reaction Engineering

Panelists: M. Burka, M.P. Dudukovic, J.A. Moulijn, A. Oroskar, L.D. Schmidt

8:50-9:00 am ISCRE 19 Introduction [Adams]

9:00-9:05 am Transition to Parallel Sessions

9:05-9:55 am Parallel Oral Sessions

17. Catalytic Reactions and Reactors B [Monroe]
18. Reactor Dynamics and Control [Parlor F]
19. Advances in Industrial Processes B [Parlor H]
20. Multiphase Reactors, Including Pharmaceutical Reactions B [Adams]

9:55-10:10 am Coffee Break

10:10 am-12:15 pm Parallel Oral Sessions (Continued following Coffee Break)

17. Catalytic Reactions and Reactors B [Monroe]
18. Reactor Dynamics and Control [Parlor F]
19. Advances in Industrial Processes B [Parlor H]
20. Multiphase Reactors, Including Pharmaeutical Reactions B [Adams]

Session 17. Catalytic Reactions and Reactors B

Wednesday, June 9, 9:20 am-12:15 pm [Monroe]

Chair: J.A. Moulijn; Co-Chair: R. V. Chaudhari

9:05-9:30 Catalytic Reactions and Reactors (invited lecture)
F. Keil. University of Hamburg-Harburg, Hamburg, Germany

9:30-9:55 Catalytic Partial Oxidation of Higher Hydrocarbons: Mixtures and Computational Modeling
R. Subramaniam, J.J. Krummenacher, G.J. Panuccio and L.D. Schmidt. University of Minnesota, Minneapolis, MN

9:55-10:10 am Coffee Break

10:10-10:35 Direct Gas-Phase Epoxidation of Propene with Nitrous Oxide over Modified Silica Supported FeO_x Catalysts
E. Ananieva and A. Reitzmann, University of Karlsruhe (TH), Germany

10:35-11:00 Enhanced Catalyst Performance Using Integrated Structured Functionalities
M. Gruenewald and D.W. Agar, University of Dortmund, Dortmund, Germany

11:00-11:25 Compensating and Predicting Catalyst Deactivation at High-temperature Conditions through Reverse-flow Reactor Operation
G. Veser, A. Mitri and D. Neumann. University of Pittsburgh, PA

11:25-11:50 Iron Zeolites for Valorization of Propane and N_2O via Oxidative Conversions. Catalyst and Reactor Design for Efficient Process Operation
A. Gallardo-Llamas, C. Daniel, C. Mirodatos and J. Perez-Ramirez. Norsk Hydro–Agri Research Centre, Porrsgrun, Norway

11:50-12:15 The Pseudo-equilibrium Effect Caused by Water on Cation Exchange Resin Catalyzed Reactions
E. du Toit and W. Nicol. University of Pretoria, South Africa

Session 18. Reactor Dynamics and Control

Wednesday, June 9, 9:20 am-12:15 pm [Parlor F]
Chair: M. Marek; Co-Chair: R.M. Koros.

9:05-9:30 Challenges in and Opportunities from Hierarchical Multiscale Simulation for Catalyst Design and Reactor Optimization and Control (invited lecture)
D. Vlachos, University of Delaware, Newark, DE

9:30-9:55 Dynamics of Transversal Hot Zones in Shallow Packed-Bed Reactors
B. Marwaha, S.S. Ram, G. Viswanathan and D. Luss, University of Houston, Houston, TX

9:55-10:10 am Coffee Break

10:10-10:35 Analysis of the Complex Nonlinear Behavior of Reacting Bubbly Flows
J.J. Wang, T. Leib and J.G. Khinast, Rutgers University, Piscataway, NJ

10:35-11:00 Low Dimensional Models for Homogeneous and Multiphase Stirred Tank Reactors
M. Bhattacharya, V. Balakotaiah and M.P. Harold, University of Houston, Houston, TX

11:00-11:25 Nonlinear Dynamics of Automobile Exhaust Gas Converters: The Role of Nonstationary Kinetics
P. Koci, V. Nevoral, M. Zahrubsky, M. Kubicek and M. Marek, Prague Institute of Chemical Technology, Czech Republic

11:25-11:50 Analysis and Design of Dynamically Coupled Multiscale Reactor Simulation Codes
E. Rusli, Y. He, T.O Drews, R.C. Alkire and R.D. Braatz, Univeristy of Illinois, Urbana, IL

11:50-12:15 Diffusion limitation in Fast Transient Experiments
D.Z. Wang, F. Li and X. Zhao, Tsinghua University, China

Session 19. Advances in Industrial Processes B

Wednesday, June 9, 9:20 -11:25 am [Parlor H]
Chair: A.R. Oroskar; Co-Chair: C.J. Pereira

9:05-9:30 Adsorption and Catalytic Reaction over FCC Catalysts in a Novel Fluidized CREC Riser Simulator
J.A. Atias and H. de Lasa, University of Western Ontario, Canada

9:30-9:55 A Model for the Hydrogenation of Aromatic Compounds during Gasoil Hydroprocessing
S. Melis, L. Erby, L. Sassu and R. Baratti, Saras Ricerche Srl, Italy

9:55-10:10 am Coffee Break

10:10-10:35 Modeling the Regeneration of Petroleum Processing Catalysts
J.L. Bixby, A. Pelekh, P. Sechrist and J. Senetar, UOP LLC, Des Plaines, IL

10:35-11:00 Hydroconversion of Model Mixtures of FCC Gasoline over Metal-Zeolite Catalysts. Reaction Study and Mathematical Modeling.
E. Ocaranza, H. Gonzalez and J. Ramirez, UNICAT, Facultad de Qu_mica, UNAM, Mexico

11:00-11:25 Precipitation in Industrial Bubble Column for Production of Sodium Bicarbonate: Modeling and Experimental Validation
B. Haut, V. Halloin, T. Cartage, N. Hirschauer and A. Cockx, Université Libre de Bruxelles, Belgium

Session 20. Multiphase Reactors, Including Pharmaceutical Reactions B

Wednesday, June 9, 9:20-11:50 am [Adams]
Chair: M. Liauw; Co-Chair: M. Al-Dahhan.

9:05-9:30 Quantification of Solids Flow in a Gas-Solid Riser: Single Radioactive Particle Tracking
S. Bhusarapu, P. Fongarland and M.P. Dudukovic, Washington University, St Louis, MO

9:30-9:55 Liquid Holdup and Pressure Drop in the Gas-liquid Cocurrent Downflow
Packed-bed Reactor under Elevated Pressures, J. Guo and M.H. Al-Dahhan, Washington University, St Louis, MO

9:55-10:10 am Coffee Break

10:10-10:35 Determination of Mass Transfer Characteristics of Co-current Two-phase Flow within Structured Packing
L. Raynal, J.-P. Ballaguet and C. Barrere-Tricca, Institut Francais du Petrole, Vernaison, France

10:35-11:00 New Insights to Trickle and Pulse Flow Hydrodynamics in Trickle-Bed Reactors using MRI
M.H.M. Lim, A. Sederman and L. Gladden, University of Cambridge, United Kingdom

11:00-11:25 Conversion Rate and Mass Transfer Limitation in Trickle Bed Reactors in Presence of a Fast Reaction
M. Banchero, L. Manna, S. Sicardi, J.G. Boelhouwer, M.I. Urseanu and G. Kwant,
Politecnico di Torino, Italy

11:25-11:50 Volumetric Mass Transfer Coefficients in Slurry Bubble Columns Operating in the Heterogeneous Flow Regime
C.O. Vandu and R. Krishna, University of Amsterdam, The Netherlands

12:15-1:15 **Lunch Break**

1:15-2:55 Parallel Oral Sessions

21. Multiphase Reactors, Including Pharmaeutical Reactions C [Adams]
22. Environmental Reaction Engineering B [Parlor H]
23. Novel Reactors and Processes C [Monroe]

Session 21. Multiphase Reactors, Including Pharmaceutical Reactions C

Wednesday, June 9, 1:15-2:55 pm [Adams]
Chair: G. Veser; Co-Chair: P. L. Mills

1:15-1:40 Comparison of a Stirred Tank Batch Reactor and a Trickle Bed Reactor for the Hydrogenation of p-toluidine
K.T. Hindle, S.D Jackson and G. Web, University of Glasgow, United Kingdom

1:40-2:05 A Comparison of a Batch Recycle Reactor and an Integral Reactor with Fines for Scale-Up of an Industrial Trickle Bed Reactor from Laboratory Data
D.A. Hickman, M. Weidenbach and D.P. Friedhoff, The Dow Chemical Company, Midland, MI

2:05-2:30 Analysis of the Performance of Single Capillary and Multiple Capillary (monolith) Reactors for the multiphase Pd-catalysed Hydrogenation of 2-butyne-1,4-diol
R. Natividad, K. Nuithitikul, J. Wood and S. Raymahasay, University of Birmingham, United Kingdom

2:30-2:55 Selective Hydrogenation of Cinnamaldehyde in Biphasic System Catalysed by Chlorotris (m-trisulfonato triphenylphosphine) Rhodium (I) Complex, RhCl(TPPTS)3
K. Nuithitikul and J.M. Winterbottom, University of Birmingham, United Kingdom

Session 22. Environmental Reaction Engineering B

Wednesday, June 9, 1:15-2:55 pm [Parlor H]
Chair: M.P. Harold; Co-Chair: M. Goto

1:15-1:40 Optimization, Characterization and Evaluation of Pillared Laponite Clay Based Fe-nanocomposite for Photo Fenton Degradation of Acid Black 1
O. Sum, J. Feng, X. Hu and P.-L. Yue, Hong Kong University of Science and Technology, Hong Kong, China

1:40-2:05 From a Fixed Bed Ag-alumina Catalyst to a Modified Reactor Design: How to Enhance the Crucial Heterogeneous-homogeneous Reactions in HC-SCR
K. Arve, E.A. Popov, K. Eranen, F. Klingstedt, J. Eloranta, M. Ronnholm and D.Y. Murzin, Åbo Akademi University, Åbo/Turku, Finland

2:05-2:30 Honeycomb Monolith Activated Carbon Catalyst for Simultaneous SO_2 and NO Removal at Low Temperatures
Y. Wang and Z. Liu, Institute of Coal Chemistry, Taiyuan, China

2:30-2:55 Catalytic Wet Oxidation of Ethylene Glycol: Kinetics of Reaction on a CuO-MnOx Catalyst
A.M.T. Silva and R.M. Quinta-Ferreira, University of Coimbra, Coimbra, Portugal

Session 23. Novel Reactors and Processes C

Wednesday, June 9, 1:15 – 2:55 pm [Monroe]
Chair: A. Renken; Co-Chair: G. W. Roberts

1:15-1:40 Residence Times and Mixing of a Novel Continuous Oscillatory Flow Meso Reactor
N.M. Reis, A.A. Vicente, J.A. Teixeira and M.R. Mackley, University of Minho, Braga, Portugal

1:40-2:05 Performance of the Monolithic Stirrer Reactor: Applicability in Multi-phase Applications
I. Hoek and A.I. Stankiewicz and J.A. Moulijn, Delft University of Technology, Delft, The Netherlands

2:05-2:30 A Novel Continuous Homogeneous Catalytic Process for Fluorous Biphasic Systems
E. Perperi, Y. Huang, G.Manos, P. Angeli, D.A. Adams, C.R. Mathison, E.G. Hope and D.J. Cole-Hamilton, University College, London, United Kingdom.

2:30-2:55 Optimization of Multiple frequency Sonochemical Reactors
A. Prabhu, P.R. Gogate and A.B. Pandit, University of Mumbai, Mumbai, India

3:00 pm **Conference Adjourns**

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