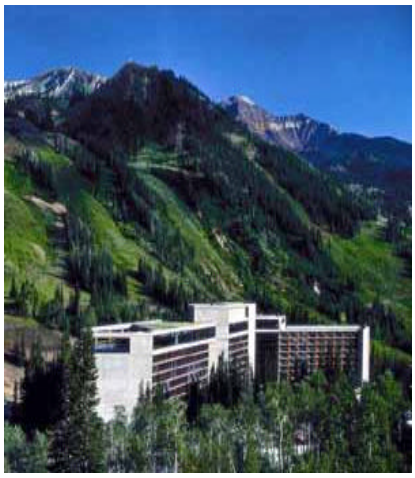
Tenth International Conference
on
Properties and Phase Equilibria
for
Product and Process Design



May 16-21, 2004

Snowbird, Utah, USA

Snowbird Ski and Summer Resort
Highway 210, Entry 4 Cliff Lodge
Snowbird, UT 84092-9000
Guest Telephone (801) 933-2222
Guest Fax (801) 933-2119

PPEPPD 2004

Final Program

http://www.engconfintl.org/4aa.html
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Engineering Conference International
6 Metro Tech Center
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Vice Chair: **Peter Cummings**, Vanderbilt University and Oak Ridge National Laboratories, USA
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Logistical Arrangements / Information

Engineering Conferences International
6 MetroTech Center
Brooklyn, NY 11201, USA
Phone: 1-718-260-3743, Fax: 1-718-260-3754
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LOCATION

Snowbird is a mountain conference resort located 25 miles from Salt Lake City in the Wasatch-Cache and Uinta National Forests of Utah. Nestled amid the rugged beauty and spectacular scenery of Little Cottonwood Canyon, Snowbird provides the perfect setting for our conference – outstanding meeting facilities, comfortable lodging, superior cuisine, good off-season rates, and an international airport only 29 miles away. The conference will be held in the Cliff Lodge and Conference Center, which features a large ballroom for our general session and offers state of the art audiovisual capabilities. The resort boasts a world-class spa with health club, whirlpools and pool, and is 10-15 minutes away from a racket and fitness club that was rated club of the year by the U. S. Tennis Association. Other activities include hiking, swimming, shopping, a large game room, and co-generation plant tours.

LODGING

All participants will be housed at Snowbird Resort's Cliff Lodge. Their contact information is

Snowbird Ski and Summer Resort
Highway 210, Entry 4 Cliff Lodge
Snowbird, UT 84092-9000
Guest Telephone (801) 933-2222
Guest Fax (801) 933-2119

JOHN M. PRAUSNITZ AWARD

The third John M. Prausnitz Award for Outstanding Achievement in applied thermodynamics will be awarded to Professor **David A. Kofke** of the State University of New York at Buffalo.

CONFERENCE REGISTRATION DESK

Participants may pick up their badge and registration materials, including a list of participants, at the Meeting Registration and Information Area, which is outside the Meeting Hall (Ballrooms 1 and 2).
Registration for the Meeting is: Sunday, May 16, 3:00 – 7:00 PM

PROCEEDINGS

All presentations will be distributed on CD-ROM to the Conference participants at registration. All papers will be refereed for publication and acceptable papers will be published in a special issue of Fluid Phase Equilibria.

POSTERS

Traditionally at the PPEPPD conferences, the majority of the presentations will be in the form of posters. For that purpose, three poster sessions are planned. The poster boards will be 4'(height) x 8'(width). They can accept velcro and/or push pins. Authors should attractively arrange their material and ensure that it is legible at a distance of 2 m.

ORAL PRESENTATIONS

Standard AV equipment includes a computer projector and an overhead projector. If you plan a PowerPoint or similar presentation and do not wish to bring a laptop, we will have one on-site. It is strongly recommended that speakers using a computer projector arrive at their sessions early to test out the equipment.

INSURANCE

Participants are advised to take out insurance as they deem necessary. The Organizers of the Conference and Engineering Conferences International cannot accept any responsibility for personal accidents or damage to private property.

WEATHER

Snowbird is located in the mountains. The climate in mountain regions can change rapidly. Please be prepared for warm sunny days, and bring a jacket for chilly evenings.

INTERNET FACILITY

There will be wireless Internet access in specific areas.

BUSINESS CENTER INFORMATION

Computer and Internet Use -- $10.00 per hour, First 15 minutes are complimentary.

TRANSPORTATION

To arrange for transportation from the airport, participants can visit the web site for Canyon Transportation at www.canyontransport.com or call (801) 255-1841 or (800) 255-1841 for reservations. The cost of a roundtrip ticket to Cliff Lodge, if made in advance, is $44. If reservations are made at the airport desk, the cost is $27 one way and $50 roundtrip. Buses run every 15-30 minutes.

SUMMARY OF DEADLINES

July 31, 2004 Submission of revised manuscripts

January 1, 2005 Publication of proceedings in Fluid Phase Equilibria special issue

OPTIONAL EXCURSIONS

There are two optional conference tours on Wednesday, May 19, 2004. Option number one is Olympic Park and Venues / Historic Park City and The Majestic Rocky Mountains. Option number two is Our City's Finest Tour and The Great Salt Lake. Sign up for tours on the conference website.

Activities that can be arranged through the hotel activities desk include: a world-class spa with health club, whirlpools and pool, hiking, swimming, shopping, a large game room, and co-generation plant tours. For further information, please visit www.snowbird.com.

ABOUT THE CONFERENCE

PPEPPD 2004 is the tenth in a series of conferences held at three-year intervals since 1977 at the following locations:

1977: Asilomar, California, USA
1980: West Berlin, Germany
1983: Callaway Gardens, Georgia, USA
1986: Helsingor, Denmark
1989: Banff, Alberta, Canada
1992: Cortina d'Ampezzo, Italy
1995: Snowmass/Aspen, Colorado, USA
1998: Noordwijkerhout, The Netherlands
2001: Kurashiki, Japan

The Conference brings together academic, government and industrial researchers from many countries to focus on fundamentals and applications of physical properties and phase equilibria in a wide range of industries, such as oil, gas, chemicals, pharmaceuticals, materials, biotechnology and foods. Thermodynamics is the main source of inspiration. As in 1977, the conference will be co-organized by Engineering Conferences International, formerly United Engineering Foundation.

THE PROGRAM

The conference consists of oral sessions, poster sessions, and workshops. To mark the occasion of the tenth conference we will be focussing on the big picture in thermodynamics research today. Invited speakers have been asked to give an overview of their subject with the goal of educating the participants, as well as stimulating them to become engaged in forefront problems. Topical areas include molecular simulation, statistical thermodynamics, phase equilibria and physical properties, phase transitions and applications thereof. The focus is not only on products and processes traditionally related to the oil, gas and chemical industry but also on products and processes related to pharmaceuticals, materials, biotechnology and foods.

MEETING ROOMS/ MEALS

- The technical sessions will be held in Ballrooms 1 and 2
- All group breakfasts and lunches will be located in the Aerie Room, on the 10th Floor.
- All group dinners (except for Thursday – off-site) will be located in the Golden Cliff and Magpie Room.
- All poster sessions will be located in the Superior Room and Lobby.

TECHNICAL PROGRAM

Sunday, May 16, 2004

15:00- 19:00	Registration (Ballroom Lobby)
18:00- 19:30	Reception
19:30- 20:45	Welcome *Carol Hall,* Conference Chair
	Keynote Address *James Wei*, Princeton University, USA PARADIGMS OF CHEMICAL ENGINEERING
20:45- 22:00	Evening Social

Monday, May 17, 2004

07:00- 08:30	Breakfast
08:30- 12:00	**Technical Session I --Complex Systems:** Joe Golab (BP Amoco Chemicals Inc,USA), Marc-Olivier Coppens (Delft University of Technology, The Netherlands)
08:30- 09:10	*Alice Gast,* Massachusetts Institute of Technology, USA PROTEIN ORDERING ON LIPID MEMBRANES - BIOMIMETIC PHASE TRANSITIONS (invited)
09:10- 09:50	*Matthew Tirrell*, University of California Santa Barbara, USA FORCES BETWEEN POLYELECTROLYTE MOLECULES IN VARIOUS IONIC ENVIRONMENTS (invited)
09:50- 10:20	Coffee Break
10:20- 11:00	*Robert Prud'homme,* Princeton University, USA THREE PROBLEMS IN THE THERMODYNAMICS AND DYNAMICS OF AMPHIPHILIC SELF ASSEMBLY (invited)
11:00- 11:30	*Gerd Maurer***,** University of Kaiserslautern, Germany VAPOR-LIQUID EQUILIBRIUM IN SYSTEMS (WATER + ORGANIC SOLVENT + SALT) AT LOW WATER CONCENTRATIONS BUT HIGH RATIOS OF SALT TO WATER: EXPERIMENTAL RESULTS AND MODELING (contributed)
11:30- 12:00	*Fernando Escobedo,* Cornell, USA SIMULATION OF NOVEL LIQUID-CRYSTALLINE BEHAVIOR IN COLLOIDAL AND POLYMERIC SYSTEMS (contributed)
12:00- 13:30	Lunch
14:00- 16:00	**Workshops** **I *Pharmaceutical and Biotechnology Industries: Foundations, Fundamentals and Futures*** Steven Drew (Merck - retired), Beth Junker (Merck) **II *How to migrate your PP software to CAPE-OPEN standard and benefit from it*** Kerry Irons (Dow Chemical), Nicolas von Solms (Technical University of Denmark)-Jean-Charles de Hemptinne (Institut Francais du Petrole).

16:00- 18:00	**Poster Session I** (Superior Room and Lobby and Maybird or Wasatch [based on availability])
	Session Chair: Howard Wilson (ConocoPhillips, USA)
18:00- 19:30	Dinner
19:30- 22:00	**Technical Session II -- Molecular Simulations:** Doros Theodorou (National Technical University of Athens,Greece), Peter Cummings (Vanderbilt University,USA)
19:30- 20:10	*Daan Frenkel*, FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands CONTROLLING HETEROGENEOUS CRYSTAL NUCLEATION (invited)
20:10- 20:30	Break
20:30- 21:00	*Ioannis Economou***,** NRCPS "Demokritos", Greece MOLECULAR SIMULATION OF STRUCTURE, THERMODYNAMIC AND TRANSPORT PROPERTIES OF POLYMERIC MEMBRANE MATERIALS FOR HYDROCARBON SEPARATION (contributed)
21:00- 21:30	*Juan de Pablo*, University Wisconsin, USA MOLECULAR MODELING OF THE COLLAPSE BEHAVIOR OF POLYMER NANOSTRUCTURES (contributed)
21:30-22:30	Evening Social

Tuesday, May 18, 2004

07:00- 08:30	Breakfast
08:30- 12:00	**Technical Session III: Phase Equilibria and Properties: Modeling and Experiments:** Ludo Kleintjens (Royal DSM, The Netherlands), Bob Heidemann (University of Calgary,Canada)
08:30- 09:10	*Cor Peters*, Technical University of Delft, The Netherlands FROM PHENOMENOLOGICAL OBSERVATIONS IN PHASE BEHAVIOR TOWARDS APPLICATIONS IN CHEMICAL ENGINEERING (invited)
09:10- 09:50	*Eduardo Filipe*, Instituto Superior Técnico, Portugal ALKANES + PERFLUOROALKANES = SEMIFLUORINATED ALKANES! (invited)
09:50- 10:20	Coffee Break
10:20- 10:50	*John Shaw*, University of Alberta, Canada ASPHALTENE PHASE BEHAVIOR (contributed)
10:50- 11:20	*Walter Chapman*, Rice University, USA PHASE BEHAVIOR OF POLAR AND ASSOCIATING SOLVENTS AND POLYDISPERSE COPOLYMERS WITH MULTIPLE FUNCTIONAL GROUPS USING POLAR SAFT (contributed)
11:20- 11:50	*Raymond French*, Shell Global Solutions, USA PHASE EQUILIBRIA OF ETHANOL-FUEL BLENDS (contributed)
12:00- 13:30	Lunch (on own)
13:30- 15:00	Free time, or **Vision 2020 Workshop** (Ballroom 1 with Option to Open 2): Opportunities for Collaboration: Industry, University, Government, *Tyler Thompson*, Dow USA Featured Presentation: ESTIMATING THERMODYNAMIC PROPERTIES IN CURRENT PROCESS AND PRODUCT DEVELOPMENT *Martin Schiller* (Dupont), *Joan Cordiner*, (Syngenta), *Michael Kleiber* (Siemens-Axiva), *Petr Kolar* (Mitsubishi Chemical)
15:00- 16:00	J. M. Prausnitz Award Lecture *David Kofke*, University Buffalo, USA FREE ENERGY AND ALL THAT

16:00- 18:00	**Poster Session II** (Superior Room and Lobby and Maybird or Wasatch [based on availability])
	Session Chair: Hiroshi Inomata (Tohoku University, Japan)
18:00- 19:30	Dinner
19:30- 22:00	**Technical Session IV: Thermoinformatics:** Harpreet Gulati (Invensys Simsci Esscor, USA), Suphat Watanasari (Aspen Technology, Inc., USA)
19:30- 19:40	*Harpreet Gulati,* Invensys Simsci-Esscor INTRODUCTION
19:40- 20:20	*James Olson*, Dow, USA THERMOINFORMATICS NEEDS IN THE CHEMICAL INDUSTRY (invited)
20:20- 21:00	*Michael Frenkel*, NIST, USA THERMODYNAMIC DATA ENGINE FOR THE 21st CENTURY: COMPREHENSIVE DATA STORAGE FACILITIES, PLATFORM-INDEPENDENT DATA COMMUNICATIONS, AND ON-DEMAND DATA EVALUATION AND PREDICTION EXPERT SYSTEMS (invited)
21:00- 21:20	Break
21:20- 22:00	*Paul Mathias***,** Aspentech , USA APPLIED THERMODYNAMICS IN CHEMICAL TECHNOLOGY: CURRENT PRACTICE AND FUTURE CHALLENGES (invited)
22:00-23:00	Evening Social

Wednesday May 19, 2004

07:00- 08:30	Breakfast
08:30-12:00	**Technical Session V: Green Engineering/ Sustainability:** Ken Marsh (University of Canterbury, New Zealand), Ray French (Shell, USA)
08:30- 09:10	*Ruben Carbonell,* North Carolina State University, USA NOVEL ENVIRONMENTALLY BENIGN PROCESSES FOR MICROELECTRONICS USING HIGH PRESSURE FLUIDS (invited)
09:10- 09:50	*Joan Brennecke,* University of Notre Dame, USA IONIC LIQUIDS AND GASES (invited)
09:50- 10:10	Coffee Break
10:10- 10:50	*Katsuto Otake,* National Institute Advanced Industrial Science &Technology, Japan FOR THE DEVELOPMENT OF NEW ALTERNATIVES. - CRITICAL PARAMETERS MEASUREMENT (invited)
10:50- 11:30	*Constantinos Vayenas*, University of Patras, Greece THERMODYNAMICS OF ADSORBED SPECIES AND THE DOUBLE LAYER APPROACH TO CATALYSIS (invited)
11:30- 12:00	*Petr Kolar,* Mitsubishi, Japan PREDICTION OF GAS SOLUBILITY IN BATTERY FORMULATIONS (contributed)
12:00- 13:30	Lunch (on own)
13:30- 17:30	Optional Excursions – See conference bulletin board for descriptions and information
18:00- 19:30	Dinner
19:30- 20:50	**Technical Session VI: Product Engineering for the Life Sciences Industry:** Mauricio Futran (Bristol Myers Squibb, USA), Sabine Enders (Dow, Germany)
19:30- 20:10	*Michael Thien*, Merck, USA OPPORTUNITIES FOR PREDICTIVE METHODS IN THE PHARMACEUTICAL INDUSTRY (invited)

20:10- 20:50	*Theodore Randolph*, University of Colorado, USA PROTEIN AGGREGATION- CONTRIBUTIONS FROM CONFORMATIONAL STABILITY AND COLLOIDAL STABILITY (invited)
20:50- 22:50	**Poster Session III** (Superior Room and Lobby and Maybird or Wasatch [based on availability])
	Session Chair: Lloyd Lee (University of Oklahoma, USA)

Thursday, May 20, 2004

07:00- 08:30	Breakfast
08:30- 12:00	**Technical Session VII Solid Fluid Equilibria:** Theo de Loos (Delft University of Technology, The Netherlands), Costa Tsonopoulos (ExxonMobil-retired, USA)
08:30- 09:10	*Costas Pantelides*, Imperial College London, UK AB INITIO PREDICTION OF CRYSTAL STRUCTURE(invited)
09:10- 09:50	*Charles Zukoski*, University of Illinois, USA EQUILIBRIUM AND KINETICALLY TRAPPED STATES IN COLLOIDAL SUSPENSIONS (invited)
09:50-10:20	Coffee Break
10:20-10:50	*Dendy Sloan*, Colorado School Mines, USA A CHANGING HYDRATE PARADIGM – FROM AVOIDANCE TO RISK MANAGEMENT (contributed)
10:50-11:20	*Peter Monson*, University of Massachusetts, USA SOLID-FLUID EQUILIBRIUM FOR ORGANIC MOLECULES: UNDERSTANDING THE LINK BETWEEN MOLECULAR STRUCTURE AND PHASE DIAGRAMS (contributed)
11:20-11:50	*Amyn Teja*, Georgia Tech, USA SOLID-LIQUID EQUILIBRIA IN AQUEOUS AMINO ACID SYSTEMS (contributed)
12:00-13:30	Lunch
13:30-17:30	**Technical Session VIII: Polymers:** Karel Aim (Institute of Chemical Process Fundamentals,Czech Republic), Jack Heidman (ExxonMobil, USA)
13:30-14:10	*Sharon Glotzer*, University of Michigan, USA SELF-ASSEMBLY OF TETHERED NANO BUILDING BLOCKS (invited)
14:10-14:50	*Hans Fraaije*, Leiden University, The Netherlands PROSPECTS FOR COMPUTATIONAL SOFT NANOTECHNOLOGY (invited)
14:50-15:20	Break
15:20-16:00	*Gabriele Sadowski*, University of Dortmund, Germany

	THERMODYNAMIC MODELLING OF COMPLEX SYSTEMS USING PC-SAFT (invited)
16:00-16:30	*Sanat Kumar*, Rensselaer Polytechnic, USA PHASE TRANSITION IN THIN POLYMER FILMS (contributed)
16:30-16:40	*Doros Theodorou*, National Technical University of Athens, Greece INVITATION TO PPEPPD 2007
18:00	Board buses for transfer to Log Haven. Log Haven is a beautiful log mansion, serenely nestled among pines, waterfalls and wildflowers, perfectly showcasing Utah's Wasatch National Forest.
18:45	Arrive at Log Haven Please get a drink and find a seat in the outside auditorium as soon as possible.
19:00- 19:30	Performance by Nino Reyes and the "Z-Tribe" This group is comprised of Nino Reyos, a member of the Northern Ute and Laguna Pueblo Indian Natives who dances and plays the flute, and members of other Tribes.
19:30- 21:00	Dinner Buffet
21:00- 22:00	Social
22:00- 22:15*	Board Buses
22:45	Return to Snowbird

* The first bus will depart as soon as it is full.

Friday, May 21, 2004

07:00- 08:30	Breakfast
08:30-12:00	**Technical Session IX: Future Directions:** John O'Connell (University of Virginia, USA), Tyler Thompson (Dow, USA)
08:30- 09:10	*Stanley Sandler*, University of Delaware, USA MOLECULAR SIMULATION WITH QUANTUM-BASED INTERACTION POTENTIALS: THE NEXT STEP (invited)
09:10- 09:50	*Geoffrey Maitland*, Schlumberger Cambridge Research, UK IMPROVING HYDROCARBON RECOVERY: CHALLENGES FOR PROCESSES, MEASUREMENTS AND MODELS (invited)
09:50- 10:20	Coffee Break
10:20- 11:00	*Enrico Drioli*, Institute Membrane Technology (ITM-CNR), Italy THE ARTIFICIAL MEMBRANES AS INTERPHASES FOR MOLECULAR SEPARATIONS, CHEMICAL CONVERSIONS, MASS AND ENERGY TRANSFER (invited)
11:00- 11:30	Panel Discussion
11:30- 11:45	Closing Remarks
12:00	Lunch (on own) and Departure

Poster Session I
Monday, May 17, 2004 16:00 – 18:00

1. NUCLEATION AND GROWTH KINETIC EFFECTS ON PARTICLE SIZE DISTRIBUTIONS

   Byung S Choi and Terry A Ring
   (University of Utah)

2. GENERALISED VIRIAL EQUATION OF STATE FOR NATURAL GAS SYSTEMS

   Jorge F Estela-Uribe and Juliana Jaramillo
   (Universidad Javeriana Cali)

3. EXPERIMENTAL AND SIMULATION STUDIES ON THE MESO STRUCTURES OF GEMINI (12-3-12,2BR-)-SDS-H2O TERNARY

   Ying Hu, Honglai Liu, Bingqiang Wang, and Yazuo Shang
   (East China University of Science and Technology)

4. SIMULATION OF THE MACROSCOPIC PITCH OF CHIRAL NEMATIC LIQUID CRYSTALLINE MATERIALS

   George Jackson, and Szabolcs Varga
   (University of Veszprém)

5. CALCULATION OF PHASE EQUILIBRIA IN THREE-PHASE SYSTEM

   O. O. Kochubey, E K. Bevza, and D V Yevdokymov
   (Dniepropetrovsk National University)

6. RECENT APPLICATIONS OF THE CUBIC-PLUS-ASSOCIATION (CPA) EQUATION OF STATE TO INDUSTRIALLY IMPORTANT SYSTEMS

   Georgios M Kontogeorgis, Samer Derawi,
   Michael L Michelsen, and Erling H. Stenby
   (Technical University of Denmark)

7. COMPUTER-AIDED AND PREDICTIVE MODELS FOR DESIGN OF CONTROLLED RELEASE OF PESTICIDES

   Núria Muro Suñé, Jorge Marrero, Rafiqul Gani,
   Gordon Bell[1], and Ian Shirley[1]
   (CAPEC, KT-DTU, 1: SYNGENTA)

8. COOPERATIVITY OF BINDING OF MULTIPLY ANCHORED POLYMER CHAINS TO LIPOSOME SURFACES

   Debra Auguste and Robert K Prud'homme,
   (Princeton University)

9. INTERACTIONS OF PHOSPHOLIPID BILAYERS WITH ALCOHOLS AND DISACCHARIDES INVESTIGATED BY ATOMISTIC SIMULATION

   Roland Faller
   (UC Davis)

10. STABILITY, EQUILIBIRUM AND MECHANICAL PROPERTIES OF PHOSPHOLIPID BILAYERS

Amadeu K Sum and Juan J de Pablo
(University of Wisconsin, Madison)

11. GROUP CONTRIBUTION BASED PROCESS FLOWSHEET SYNTHESIS, DESIGN AND MODELLING

Loïc d'Anterroches and Rafiqul Gani
(Technical University of Denmark)

12. COMBINING MOLECULAR DYNAMICS AND CHEMICAL PROCESS SIMULATION USING THE SPEAD METHOD

J. Richard Elliott, Z. Gerek Nevin, Neil Gray, and John Guy
(The University of Akron)

13. CARBON NANOTUBES AS MOLECULAR CHANNELS

Shekhar Garde[1], Amrit Kalra [2], and Gerhard Hummer[3]
(1: Renssepaer Polytechnic Institute, 2: Massachusetts Institute of Technology, 3: NIDDk, National Institute of Health)

14. EXPERIMENTAL THERMODYNAMIC DATA AND FUNDAMENTAL EQUATIONS OF STATE FOR THE BUTENE ISOMERS

Christian Ihmels [1], Eric Lemmon [2], Kai Fischer [1], and Jürgen Gmehling [3]
(1: Laboratory for Thermophysical Properties, 2: National Institute of Standards and Technology, 3: University of Oldenburg)

15. FLUIDS CONFINED IN CARBON NANOTUBES: INSIGHTS FROM MOLECULAR SIMULATIONS

Jianwen Jiang and Stanley I Sandler
(University of Delaware)

16. MOLECULAR RECOGNITION AND ADSORPTION IN NANOSTRUCTURED MATERIALS: GAS STRUCTURE AND SENSING IN STARBURST DENDRIMERS

Lloyd L Lee and David Scott Wilson
(University of Oklahoma)

17. MOLECULAR MODELING OF ION EXCHANGE IN CRYSTALLINE SILICOTITANATE MATERIALS

Edward J Maginn and James P Larentzos
(University of Notre Dame)

18. GAS SOLUBILITY IN IONIC LIQUIDS

Gerd Maurer, J Kumelan, and Ch Hesch
(Universitaet Kaiserslautern)

19. AGGREGATION OF HEXANOL ISOMERS AND OF 2-ALKOXYETHANOLS IN *N*-HEXANE: AGGREGATION, STERIC HINDRANCE, INTER- AND INTRAMOLECULAR HYDROGEN BONDING AND VIBRATIONAL SPECTROSCOPY

John M Stubs and J. Ilja Siepmann
(University of Minnesota)

20. ADVANCED EQUATION OF STATE METHOD FOR MODELING GLYCOL GAS DEHYDRATION

Chorng H Twu, Vince Tassone, Wayne D Sim, and Suphat Watanasiri
(Aspen Technology, Inc.)

21. EQUATION FOR SELF AND MUTUAL-DIFFUSION COEFFICIENTS OF LENNARD-JONES CHAIN FLUIDS: HYDROCARBONS AND POLYMERIC SYSTEMS

Rodrigo Azevedo dos Reis [1], Ronaldode Nobrega[1], José Vladimir Oliveira[2,] and Frederico Wanderlei Tavares [3]
(1: COPPE/UFRJ, 2: URI – Campos de Erechim, 3: Universidade Federal do Rio de Janeiro)

22. A ROBUST AND EFFICIENT ALGORITHM FOR BINARY PHASE EQUILIBRIUM CALCULATIONS

Apostolos Giovanoglou, Claire S Adjiman, Amparo Galindo, and George Jackson
(Imperial College London)

23. IN SITU NEUTRON DIFFRACTION AND SPECTROSCOPIC STUDIES OF CLATHRATE HYDRATE FORMATION, DECOMPOSITION AND INHIBITION

Carolyn Ann Koh [1], Alan K Soper [2], Piers Buchanan [3], Nawaf Aldiwan [4], Jefferson L Creek[5], Angela Carstensen[5], and Robin E. Westacott[5]
(1: Colorado School of Mines, 2: Rutherford Appleton Laboratory, 3: King's College London, 4: Heriot-Watt University, 5: ChevronTexaco Exploration and Production Technology Company)

24. CALCULATION OF CRITICAL POINTS USING A REDUCTION METHOD

Dan Vladimir Nichita
(Instituto Mexicano del Petroleo)

25. KINETIC AND THERMODYNAMIC STABILITY LIMITS INVESTIGATED BY TRANSITION-MATRIX MONTE CARLO

Vincent K Shen [1] and Jeffrey R Errington [2]
(1: National Institute of Standards and Technology, 2: University at Buffalo)

26. NOVEL OPTICAL FLOW CELL FOR MEASUREMENT OF FLUID PHASE BEHAVIOUR

J P Martin Trusler [1], Nicola Riesco [2], and Mohammad S Islam [1]
(1: Imperial College London, 2: University of Valladolid)

27. SIMULATING PEO MELTS AND PEO-CO2 PHASE EQUILIBRIA USING CONNECTIVITY-ALTERING MONTE CARLO

Collin Wick and Doros N Theodorou
(National Technical University Athens)

28. APPLICATION OF THE PC-SAFT MODEL TO TER POLYMER SYSTEMS

F Barbagini and T Tiemersma
(DSM Research)

29. GLOBAL PHASE BEHAVIOR OF CHAIN MOLECULES: A COMPARISON OF FLEXIBLE AND LINEAR RIGID MODELS

Felipe J Blas [1], Amparo Galindo[2], Carlos Vega[3],
Eduardo Sanz [1], Luis G McDowell, and Enrique de Miguel
(1: Universidad de Huelva, 2: Imperial College,
3: Universidad Complutense de Madrid)

30. SPINODAL CURVES AND CRITICAL POINTS IN MIXTURES CONTAINING POLYDISPERSE POLYMERS WITH MANY COMPONENTS

Robert A. Heidemann, Ryan A Krenz, and Torben Laursen
(University of Calgary)

31. AN EXAMINATION OF THE EFFECT OF POLYDISPERSITY ON THE CLOUD CURVES OF POLYMER SOLUTIONS WITH WERTHEIM TPT1 DESCRIPTION

George Jackson [1], Patrice Paricaud[1], and Amparo Galindo[2]
(1: Vanderbilt University, 2: Imperial College London)

32. INFLUENCE OF FREE INTERFACES ON GLASSY DYNAMICS

Tushar Jain and Juan J de Pablo,
(University of Wisconsin-Madison)

33. PREDICTION AND CORRELATION OF SOLID SOLUBILITY IN SOLVENTS AND SOLVENT MIXTURES

David Bush [1], Michael J Lazzaroni[1], Malina Janakat [1], Charles A Eckert[1],
Timothy C Frank [2], Sumnesh K. Gupta[2], James D. Olson[2]
(1: Georgia Institute of Technology, 2: The Dow Chemical Company)

34. MEASUREMENT AND MODELING OF THE EQUILIBRIA BETWEEN AQUEOUS SOLUTIONS OF ELECTROLYTES AND ION EXCHANGE RESINS.

Søren Gregers Christensen and Kaj Thomsen
(Technical University of Denmark)

35. HIGH PRESSURE SOLID-FLUID AND VAPOUR-LIQUID EQUILIBRIA IN MODEL HYPERBARIC FLUIDS

Th W de Loos and J J M Machado
(Delft University of Technology)

36. PREWETTING TRANSITIONS FOR A MODEL ARGON ON SOLID CARBON DIOXIDE SYSTEM

Jeffrey R Errington,
(University at Buffalo, The State University of New York)

37. EVAPORATIVE DEHYDRATION OF SOFT CONTACT LENSES

F Fornasiero, J M Prausnitz, and C J Radke
(University of California Berkeley)

38. APPLICATION OF A NEW CLASS OF EQUATIONS OF STATE FOR ASSOCIATING AND POLAR FLUIDS TO METHANOL + CARBON DIOXIDE BINARY SYSTEM

Karel Aim, A Babic, and L Vlcek
(Institute of Chemical Process Fundamentals)

39. SOLUBILITY OF THIOPHENE IN SUPERCRITICAL CARBON DIOXIDE + 1-PROPANOL MIXTURES AT TEMPERATURES FROM 313 TO 363 K

Luis A Galicia-Luna, and Octavio Elizalde Solis
(Instituto Politecnico Nacional)

40. PREDICTING THE THERMODYNAMIC PROPERTIES AND SURFACE TENSION OF FLUIDS USING THE SAFT-VRX EQUATION OF STATE

Clare McCabe, Sergei B Kiselev, Honggang Zhao, and Lixin Sun
(Colorado School of Mines)

41. COMPARISON OF MUTUAL DIFFUSION COEFFICIENT DATA IN A TERNARY LIQUID MIXTURE OBTAINED BY VARIOUS EXPERIMENTAL TECHNIQUES

Jochen Winkelmann, and Dimitry A Ivanov
(University Halle-Wittenberg Institute Physical Chemistry)

42. MOLECULAR SIMULATIONS OF THE LIQUID-LIQUID INTERFACE IN PARTIALLY MISCIBLE MIXTURES

Richard L Rowley, Eric Carlson, Kent Wardle and Douglas Henderson
(Brigham Young University)

Poster Session II
Tuesday, May 18, 2004 16:00 – 18:00

43. A NEW MODEL TO CORRELATE AND TO PREDICT SHEAR VISCOSITY OF DENSE FLUIDS

Luiz Antonio Ferreira Coelho
(Universidade do Estado de Santa Catarina)

44. HIGH-PRESSURE LIQUID-VAPOR AND LIQUID-LIQUID-VAPOR EQUILIBRIA OF TWO BINARY IONIC LIQUID SYSTEMS

Alireza Shariati, Karin Gutkowski, and Cor J Peters
(Delft University of Technology)

45. PREDICTION OF INTERNAL STRUCTURE AND PROPERTIES IN BINARY AND TERNARY FLUID INTERFACIAL SYSTEMS:

Jochen Winkelmann, Heike Kahl, and Matthias Mecke
(University Halle-Wittenberg Institute of Physical Chemistry)

46. UNIFIED DENSITY FUNCTIONAL THEORY OF COMPLEX FLUIDS

Jianzhong Wu
(University of California, Riverside)

47. LIQUID PHASE BEHAVIOR FOR IONIC LIQUIDS OF DIFFERENT CATION TYPES WITH ALCOHOLS

Jacob M Crosthwaite, Mark J Muldoon, Sudhir N V K Aki,
Edward J. Maginn, and Joan F. Brennecke
(University of Notre Dame)

48. WATER-MEDIATED INTERACTIONS RELEVANT TO PROTEIN STRUCTURE AND STABILITY: UNDERSTANDING PRESSURE EFFECTS ON PROTEINS

Tuhin Ghosh[1], Angel E Garcia[2], and Shekhar Garde[1]
(1: Rensselaer Polytechnic Institute, 2: Los Alamos National Laboratory)

49. MOLECULAR SIMULATION OF BIOMETALS ADSORPTION ON ION TRANSPORTER PROTEINS

Christian Lastoskie, Wei Shi, and Ann Marie Sastry
(University of Michigan)

50. AQUEOUS PROTEIN-PROTEIN POTENTIAL OF MEAN FORCE: PHASE DIAGRAMS AND ION SPECIFICITY

Frederico Wanderley Tavares[1], and John M Prausnitz[2]
(1: Universidade Federal do Rio de Janeiro, 2: University of California)

51. PREDICTION OF THERMODYNAMIC PROPERTIES OF HEAVY HYDROCARBONS BY MONTE CARLO SIMULATION

Goktug Ahunbay[1], Spyridon Kranias[2],
Véronique Lachet[3], and Philippe Ungerer[3]
(1: Laboratoire de Chimie Physique,
2: Université Paris-Sud, 3: Institut Français du Pétrole)

52. A FREE-VOLUME TERM BASED ON THE VAN DER WAALS PARTITION FUNCTION FOR THE UNIFAC MODEL

Ronald P Danner, D.C. Kannan, and J.L. Duda
(The Pennsylvania State University)

53. SELF-DIFFUSION COEFFICIENTS OF IONS IN MODEL ELECTROLYTE SOLUTIONS BY SMART BROWNIAN DYNAMICS SIMULATION

Guang-Hua Gao, Hong-Bing Shi, and Yang-Xin Yu
(Tsinghua University)

54. A MOLECULAR DYNAMICS STUDY OF LOCAL PROPERTIES AND DYNAMICS OF SOLUTION STRUCTURE OF SUPERCRITICAL WATER - METHANOL SYSTEM

Tetsuo Honma[1], Takayuki Saito[1], Hiroshi Inomata[2], and Yoshio Sato[1]
(Hachinohe National College of Technology, 2: Tohoku University)

55. VAPOR-LIQUID EQUILIBRIA FOR CO2-FERMENTATION ALCOHOL MIXTURES - APPLICATION OF NEW GROUP CONTRIBUTION EQUATION OF STATE FOR ISOMERIC COMPOUNDS

Hiroshi Inomata, Akihiro Kondo, and Hideki Kakehashi
(Tohoku University)

56. ETOMICA: A JAVA-BASED DEVELOPMENT ENVIRONMENT FOR MOLECULAR SIMULATIONS

David A Kofke, Jayant Singh, Sang-kyu Kwak, and Di Wu
(University at Buffalo)

57. EXTENDING THE HNC INTEGRAL EQUATION THEORY THROUGH DIRECT EVALUATION OF BRIDGE DIAGRAMS USING MOLECULAR SIMULATION

Sang-kyu Kwak and David A Kofke
(University at Buffalo)

58. SIMULATION OF THE SOLUBILITY OF CARBON DIOXIDE AND HYDROGEN SULFIDE IN POLYETHYLENE MELT

Véronique Lachet and Philippe Ungerer
(Institut Français du Pétrole)

59. MONTE CARLO SIMULATIONS OF BIOMOLECULE- AND POLYMER-DIRECTED NANOSCALE ASSEMBLY

Monica Hitchcock Lamm[1], Ting Chen[2], and Sharon C Glotzer[2]
(1: Iowa State University, 2: University of Michigan)

60. EXAMINATION OF HENRY'S CONSTANT FOR CARBON DIOXIDE IN WATER BY MONTE CARLO SIMULATIONS

Martin Lisal[1], William R Smith[2], and Karel Aim[1]
(1: E. Hala Lab of Thermo, ICPF, AS CR, 2: Un. of Guelph)

61. AB INITO STUDY ON AQUEOUS MGCL2 AND CACL2 SOLUTIONS AT HYDROTHERMAL AND SUPERCRITICAL RANGE

Lu Xiaohua, Hao Ding, Yu Zhu, and Jun Wang
(Nanjing University of Technology)

62. CONCENTRATION-DEPENDENT DIFFUSION COEFFICIENTS FROM A SINGLE EXPERIMENT USING MODEL-BASED RAMAN SPECTROSCOPY

Andre Bardow, Volker Goeke, Hans Juergen Koss, Klaus Lucas, and Wolfgang Marquardt
(Lehrstuhl fuer Prozesstechnik, RWTH Aachen University)

63. PHASE BEHAVIOR STUDIES OF A PERFLUOROPOLYETHER IN HIGH PRESSURE CARBON DIOXIDE

Teresa Casimiro[1], Alireza Shariati[2], Cor J Peters[2], Manuel Nunes da Ponte[1], and Ana Aguiar-Ricardo[1]
(1: Universidade Nova de Lisboa, 2: Delft University of Technology)

64. PHASE EQUILIBRIA OF N-PERFLUOROALKANE/CARBON DIOXIDE/N-ALKANE TERNARY MIXTURES

Coray Colina and Keith E Gubbins
(North Carolina State University)

65. PHASE BEHAVIOR OF SOYBEAN AND OLIVE OILS IN COMPRESSED PROPANE AND N-BUTANE

José Vladimir de Oliveira, Marcelo Lanza, Débora de Oliveira, Papa Mattar Ndiaye, and Cláudio Dariva
(URI-Campus de Erechim)

66. ON THE INFINITE DILUTION PROPERTIES OF N-ALKANES IN NEAR CRITICAL WATER AND THEIR RELATION TO PHASE EQUILIBRIA

Clare McCabe[1], Amparo Galindo[2], and Peter T. Cummings[3]
(1: Colorado School of Mines, 2: Imperial College London, 3: Vanderbilt University)

67. SECOND AND THIRD VIRIAL COEFFICIENTS FOR THE R41+N2O SYSTEM

Fabio Polonara[1], Giovanni Di Nicola[1], Giuliano Giuliani[1], and Roman Stryjek
(1: Università Politecnica delle Marche, 2: Polish Academy of Sciences)

68. APPLICATION OF A MODIFIED RESS PROCESS FOR POLYPROPYLENE MICROPARTICLE PRODUCTION

Cláudio Dariva[1], José Carlos Pinto[2], and José Vladimir de Oliveira[1]
(1: URI-Campus de Erechim, 2: PEQ/COPPE/UFRJ)

69. DESIGN OF SURFACES FOR PATTERN RECOGNITION USING COMPUTER SIMULATION

Arthi Jayaraman, Carol K Hall, and Jan Genzer
(North Carolina State University)

70. MOLECULAR DYNAMICS SIMULATION AND MOLECULAR THERMODYNAMIC MODEL FOR POLYAMPHOLYTE SOLUTIONS

Honglai Liu, Jian Feng, and Ying Hu
(East China University of Science and Technology)

71. AN EXAMINATION OF THE VAPOR-LIQUID PHASE BEHAVIOR OF PERFLUOROALKANE-ALKANE DIBLOCK SURFACTANTS: THEORY AND EXPERIMENT

Pedro Morgado[1], Honggang Zhao[1], Clare McCabe[1], Felipe J. Blas[2], and Eduardo J. M. Felipe[3]
(1: Colorado School of Mines, 2: Universidad de Huelva, 3: Instituto Superior Técnico)

72. EXPERIMENTAL AND SELF-CONSISTENT FIELD THEORETICAL STUDY OF STYRENE BLOCK COPOLYMER SELF-ADHESIVE MATERIALS

Doros N Theodorou[1], Kostas Ch. Daoulas[2], Alexandra Roos[3], and Costantino Creton[3]
(1: National Technical University of Athens, 2: ICE/HT-FORTH, 3: Laboratoire PCSM, ESPCI)

73. ENERGY LANDSCAPE PERSPECTIVES FOR THE PROPERTIES OF THIN FILMS

Thomas M Truskett, Jeetain Mittal, Pooja Shah, and Venkat Ganesan,
(The University of Texas at Austin)

74. MONTE CARLO SIMULATIONS OF SOLID-LIQUID PHASE DIAGRAMS FOR DIASTEREOMERIC MOLECULES

Aysa L Akad and Carol K Hall
(North Carolina State University)

75. EQUILIBRIUM AND DYNAMICS OF GAS HYDRATES

Walter G Chapman[1], Shuqiang Gao[1], Matthew Yarrison[1], Kyoo Song[1], and Waylon House[2]
(1: Rice University, 2: Texas Tech University)

76. TOWARDS DEVELOPING RELIABLE MODELS FOR ELECTROLYTE SOLUTIONS: EXTENSIONS OF THE SAFT APPROACH TO TREAT MIXED-SOLVENT SYSTEMS

Amparo Galindo[1], Birjukumar Patel[1], Patrice Paricaud[2], and Geoffrey C. Maitland[3]
(1: Imperial College London, 2: Vanderbilt University, 3: Schulmberger Cambridge Research)

77. USING MONTE CARLO TO STUDY CONCENTRATION AND TEMPERATURE EFFECTS ON SOLVATION

Collin Wick[1] and J. Ilja Siepmann[2]
(1: National Technical University Athens, 2: University of Minnesota)

78. THERMODYNAMIC METHOD FOR OBTAINING THE SOLUBILITIES OF COMPLEX MEDIUM-SIZED CHEMICALS IN PURE AND MIXED SOLVENTS

Jens Abildskov[1] and John P O'Connell[2]
(1: CAPEC, DTU, 2: University of Virginia)

79. VISCOSITY CORRELATIONS OVER A WIDE RANGE OF FLUID STATES FOR MINOR CONSTITUENT FLUIDS IN NATURAL GAS

Marcia L Huber and Arno Laesecke
(NIST)

80. A MICROWAVE RESONANT CAVITY FOR DEW POINT DETERMINATIONS

Kenneth N Marsh[1], Mohamed E Kandil[1], and Anthony R H Goodwin[2]
(1: University of Canterbury, 2: Schlumberger Oilfield Services)

81. APPLICATION TO BINARY MIXTURES OF A GROUP CONTRIBUTION SAFT EOS

Sofiane Tamouza[1], J-Philippe Passarello[2], Pascal Tobaly[2], and J-Charles de Hemptinne[1]
(1: Institut Français du Pétrole, 2: Laboratoire d'Ingénierie des Matériaux et des Hautes Pressions (C. N. R. S.))

Poster Session III
Wednesday, May 19, 2004 20:50 – 22:50

82. LIMITATIONS VS LIMITING LAWS: ADVANCED EOS MODELS FOR COMPLEX SOLUTIONS

Kenneth R Cox
(Rice University)

83. DENSE-GAS EXTRACTION: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS FOR THE FRACTIONATION OF OLIGOMERIC MATERIALS

William F Edwards and Mark C Thies
(Clemson University)

84. THREE-PHASE AND FOUR-PHASE PREDICTIONS FOR POLYETHYLENE + HYDROCARBON SYSTEMS

Robert A Heidemann[1], R A Krenz[1], and Th W de Loos[2]
(1: University of Calgary 2: Delft University of Technology)

85. GAS-EXPANDED LIQUIDS: A SYNERGY OF THEORY AND EXPERIMENT

Charu Shukla
(Georgia Institute of Technology)

86. THE IMPACT OF MULTIPHASE BEHAVIOUR ON COKE FORMATION AND CATALYST DEACTIVATION IN HYDROPROCESSING OF RESIDS

Xiaohui Zhang and John M Shaw
(University of Alberta)

87. SOLUBILITY MEASUREMENT AND PREDICTION OF CARBON DIOXIDE IN IONIC LIQUIDS

C S Lee[1], Y S Kim[1], W Y Choi[1], and K -P Yoo[2]
(1: Korea University, 2: Sogang University,)

88. PROCESS INTENSIFICATION CONCEPT APPLIED TO WASTEWATER TREATMENT

Renata Torres Pereira Pinto[1], Luiz Fernando da Lima Luz Jr[2], and Maria Regina Wolf-Maciel[1]
(1: State University of Campinas, 2: Federal University of Paraná)

89. PHASE EQUILIBRIA IN PROTEIN SOLUTIONS: FORMATION OF AN AMYLOID FIBRIL BY A PEPTIDE DERIVED FROM LYSOZYME

Wei Liu, John Prausnitz, and Harvey Blanch
(University of California at Berkeley)

90. DIAMETER AND HELICITY EFFECTS ON THE STRUCTURE AND DIFFUSION OF AQUEOUS NACL CONFINED IN NANOTUBES

Xiaohua Lu, Jun Wang, Yu Zhu, and Jian Zhou
(Nanjing University of Technology)

91. OPEN SYSTEM SIMULATION OF LLE USING GRAUDAL INSERTIONS AND GIDDS-DUHEM INTEGRATION

Timothy I Morrow and Edward J Maginn
(University of Notre Dame)

92. MESOSCALE SIMULATION OF PEPTIDE ADSORPTION ON REVERSED-PHASE CHROMATOGRAPHY MEDIA

John P. O'Connell
(University of Virginia)

93. DENSITY FUNCTIONAL THEORY APPLIED TO THERMOCHEMISTRY QUANTITY CALCULATIONS FOR PHENOL REACTIONS

Miria H M Reis, Hueder Paulo M de Oliveira, Teresa D Z Atvars, Liege F S Mascolo, and Maria Regina Wolf-Maciel
(State University of Campinas)

94. DENSITY OF STATES MONTE CARLO METHODS FOR OFF-LATTICE MOLECULAR MODELS

M Scott Shell, P G Debenedett, and A Z Panagiotopoulos
(Princeton University)

95. MOLECULAR SIMULATION STUDY OF SURFACE TENSION OF ASSOCIATING FLUIDS

Jayant Singh and David A Kofke
(University at Buffalo)

96. INTERFACIAL PHASE AND CHEMICAL EQUILIBRIA OF POLYATOMIC ASSOCIATING FLUIDS FROM INTERFACIAL-SAFT (*I*-SAFT)

Sandeep Tripathi and Walter G Chapman
(Rice University)

97. NEW ALGORITHM FOR COMPUTING HOMOGENEOUS AND HETEROGENEOUS REACTIVE AZEOTROPES

M R Wolf-Maciel, M. H. R. Reis, and L F S Mascolo
(State University of Campinas)

98. UNDERSTANDING THE INFLUENCE OF PHASE-SPACE OVERLAP IN FREE ENERGY CALCULATIONS

Di Wu and David A Kofke
(University at Buffalo)

99. SOLUBILITY OF CARBON DIOXIDE IN A MIXED SOLVENT AT ELEVATED PRESSURES

A E Mather
(University of Alberta)

100. EXPERIMENTAL TECHNIQUES FOR VAPOR PRESSURE AND VAPOR-LIQUID EQUILIBRIUM OF LOW VOLATILE COMPOUNDS

Hiroaki Nakata
(Mitsubishi Chemical Corporation)

101. PHASE BEHAVIORS OF SOLID POLYMER ELECTROLYTE/SALT SYSTEMS IN LITHIUM SECONDARY BATTERY: THE IONIC INTERACTION AND NONRANDOMNESS EFFECT

Sung Jin Pai, In Ha Kim, Young Chan Bae, and Kap Sik Kim,
(Hanyang University)

102. MODELING VAPOR-LIQUID AND LIQUID-LIQUID AQUEOUS INTERFACES WITH THE GRADIENT THEORY

Antonio Jose Queimada[1], Isabel M Marrucho[1], Georgios M Kontogeorgis[2], Christelle Miqueu[3], and João A P Coutinho[1]
(1: CICECO, Aveiro University, 2: IVC-SEP, Technical University of Denmark, 3: Université de Pau et des Pays de L'Adour)

103. PHASE EQUILIBRIA IN ASSOCIATING POLYMER SOLUTIONS WITH CO2 AS THE SOLVENT

Amyn S Teja and Ibrahim A Ozkan
(Georgia Institute of Technology)

104. MEASUREMENT AND MODELING OF VAPOR-LIQUID EQUILIBRIA AT HIGH SALT CONCENTRATIONS

Akio Tsuboi[1], Hiroaki Nakata[1], Petr Kolar[1], Peiming Wang[2], and Andre Anderko[2]
(1: Mitsubishi Chemical Corporation, 2: OLI Systems Inc.)

105. HYDROGEN SOLUBILITY OF CHEMICAL HYDROGEN RESERVING MEDIUM, AROMATIC HYDROCARBON, CYCLIC ALIPHATIC HYDROCARBON, AND THEIR MIXTURE, FOR FUEL CELL SYSTEM

Tomoya Tsuji, Yoshiko Shinya, Toshihiko Hiaki, and Naotsugu Itoh
(1: Nihon University, 2: National Institute of Advanced Industrial and Technology)

106. SENSITIVITY OF METHANE AND TETRAHYDROFURAN HYDRATE PHASE EQUILIBRIA TO SEDIMENT PORE SIZE

Douglas J Turner[1], Robert Cherry[2], and Dendy Sloan[1]
(1: Colorado School of Mines,
2: Idaho National Engineering & Environmental Lab)

107. INTERFACIAL PROPERTIES OF POLYSTYRENE IN CONTACT WITH CARBON DIOXIDE

Sabine Enders[1], Heike Kahl[2], and Jochen Winkelmann[2]
(1: Dow Chemical Company, 2: Martin Luther University)

108. THE BEHAVIOR OF PEN DECOMPOSITION IN SUPERCRITICAL WATER

Osamu Sato, Takafumi Sato, Kunio Arai, and Masayuki Shirai
(National Insititute of Advanced Industrial Science and Technology)

109. PREDICTION OF DIFFUSIVITY IN GLASSY POLYMERS USING MULTIDIMENSIONAL TRANSITION STATE THEORY

Doros N Theodorou[1] and Niki Vergadou[2]
(1: National Technical University of Athens,
2: Institute of Physical Chemistry, NRCPS 'Demokritos')

110. MEASUREMENT AND PREDICTION OF ACTIVITY COEFFICIENTS OF SOLUTES IN POLYMER SOLUTIONS USING GAS-LIQUID CHROMATOGRAPHIC METHOD AND CUBIC-PERTURBED EQUATION OF STATE WITH GROUP CONTRIBUTION METHOD

Katsumi Tochigi, Shinpei Kurita, andYuichi Okitsu
(Nihon University)

111. SELF-DIFFUSION COEFFICIENTS OF 1-BUTYL-3-METHYLIMIDAZOLIUM HEXAFLUOROPHOSPHATE WITH PULSED-FIELD GRADIENT SPIN-ECHO NMR TECHNIQUE

Tatsuya Umecky, Mitsuhiro Kanakubo, and Yutaka Ikushima
(National Institute of Advanced Industrial Science and Technology)

112. MEASUREMENT AND CORRELATION OF LIQUID-LIQUID EQUILIBRIA AND PARTITION COEFFICIENTS OF BENZOTHYOPHENE AND BENZOTHYOPHENE 1,1-DIOXIDE FOR ACETONITRILE + N-OCTANE SYSTEM

Takeshi Furuya, Souko Yamagami, Kazumasa Yazu, Ikuo Saito, and Mitsunori Makino
(National Institute of Advanced Industrial Science and Technology (AIST))

113. MEASUREMENT AND CORRELATION FOR SOLUBILITIES OF ALKALI METAL CHLORIDE IN WATER VAPOR AT HIGH TEMPERATURE AND PRESSURE

Hidenori Higashi, Yoshio Iwai, Yoshiaki Kitani, Yusuke Shimoyama, and Yasuhiko Arai
(Kyushu University)

114. SOLUBILITY CALCULATION OF SOLID COMPONENT INTO SUPERCRITICAL FLUID WITH USE OF LOCAL EXCESS DENSITY FROM FT-IR MEASUREMENT

Hiroshi Inomata, Naozumi Wada, and Kunio Arai
(Tohoku University)

115. METHANE RECOVERING FROM ITS HYDRATE WITH USING PRESSURED CO2

Masaki Ota, Yuki Abe, Masaru Watanabe, Richard Lee Smith Jr., and Hiroshi Inomata
(Tohoku University)

116. PARAMETERIZATION OF MOLECULAR-BASED EQUATIONS OF STATE

Claudio Olivera-Fuentes, Alexis Bouza, Coray M. Colina, and Sylvana Derjani
(Simon Bolivar University)

117. THERMODYNAMICS OF DENSE PHASE ACID GAS REMOVAL PROCESSES

Kwang W Won
(Fluor Enterprises, Inc.)

118. MOLECULAR THERMODYNAMICS IN THE PROTEIN-SALT SOLUTIONS

Bong Ho Chang, Young Chan Bae, and In Ha Kim
(Hanyang University)