

Accelerating Fossil Energy Technology Development Through Integrated Computation and Experimentation

Topical Conference at the 2012 AIChE Annual Meeting

**Pittsburgh, Pennsylvania, USA
28 October - 2 November 2012**

ISBN: 978-1-62276-750-2

Printed from e-media with permission by:

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



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

Copyright© (2012) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2013)

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

AIChE
3 Park Avenue
New York, NY 10016-5991

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

www.aiche.org

Additional copies of this publication are available from:

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

TABLE OF CONTENTS

Practical Membranes for CO₂ Capture	1
<i>Christina Myers, David Luebke, Wei Shi, Shan Wickramanayake, Brian Kail, Robert L. Thompson, Hunaid Nulwala</i>	
Theoretical and Experimental Approach to Nitrogen Selective Membranes	2
<i>Ekin Ozdogan, Panithita Rochana, Jennifer Wilcox</i>	
Poly(ionic liquid) Membranes for CO₂/N₂ Separation: Insight From Atomistic Simulation.....	4
<i>Weijie Fang, Zhonglin Luo, Jianwen Jiang</i>	
Multifold CO₂ Transport Property Enhancement of Interfacially Constrained Nanocomposite Membranes.....	5
<i>Lakshmi Suhasini Kocherlakota, Tiep Hoang Pham, René M. Overney</i>	
Nanocomposite Membrane of a Polymer of Intrinsic Microporosity and Zeolitic Imidazolate Frameworks for Gas Separation	6
<i>Qilei Song, Shaheen A. Al-Muhtaseb, Easan Sivanianah</i>	
Steam Stability of Layered Zeolites Suitable for Hydrogen Transport.....	8
<i>Bahman Elyassi, Xueyi Zhang, Michael Tsapatsis</i>	
Physical Aging and Carbon Dioxide Plasticization of Thin Polyetherimide Films.....	9
<i>Jianzhong Xia, Tai Shung Chung, Pei Li, Norman R. Horn, Donald R. Paul</i>	
The Design and Modeling of a Controlled Atmosphere Food Storage System Based On Membrane Technology	10
<i>Hang Yin, Na Peng, Kok Lin Chong, Glenn Lipscomb, Tai-Shung Chung</i>	
Effect of Confinement On Ionic Liquid Properties for Carbon Capture Processes	11
<i>Ruth E. Baltus, Laila Banu</i>	
Metallic Based Aqueous Amine Membranes for the Separation of Carbon Dioxide From Fossil Fuel Flue Gas.....	12
<i>Brian L. Bischoff, Lawrence E. Powell</i>	
A Comprehensive Multi-Step Description of the Permeation of Hydrogen in a Dense Metal Membrane Over a Broad Temperature Range	13
<i>Nicholas Deveau, Yi Hua Ma, Ravindra Datta</i>	
High Temperature Metal Membranes for Hydrogen Permeation without Platinum Group Metals.....	14
<i>J. Douglas Way, Colin A. Wolden, Kehinde Adeyemo, Mayur Ostwal</i>	
Long Term H₂ Permeance and Selectivity Stability of Pd and Pd-Au Large Scale Membranes in Actual Syngas Atmospheres.....	15
<i>Federico Guazzone, Jacopo Catalano, Ivan Mardilovich, Nikolas Kazantzis, Yi Hua Ma</i>	
Composite Catalytic Membranes: Enhancing H₂ Recovery Membranes by Appropriate Coupling with Water-Gas-Shift Reaction	16
<i>Elva Romero, Daejin Kim, Benjamin Wilhite</i>	
Toward a Common Method of Cost Estimation for CO₂ Capture and Storage At Fossil Fuel Power Plants	17
<i>Edward S. Rubin</i>	
Proposed Baselines and Standard Methods for Systems Analyses of Power Generation Technologies	18
<i>Michael Matuszewski</i>	
Methodology for Evaluating the Cost of Emerging CCS Technologies.....	19
<i>Abhoyjit S. Bhowan, George Booras, Ronald Schoff</i>	
A Common Modeling Framework to Evaluate and Compare the Economics of CCUS Technologies.....	20
<i>Edward S. Rubin</i>	
NETL CO₂ Injection and Storage Cost Model	21
<i>Tim Grant, Dave Morgan, Jason Valenstein, Andrea Poe, Marta Milan, Richard Lawrence</i>	
A Monte Carlo Approach for Estimating and Validating Contingencies for CCS	22
<i>Paul Worhach, Mark Woods, John Wimer</i>	
CO₂ Mineralisation Through Hydrometallurgical Leaching of Brown Coal Fly Ash	23
<i>Lian Zhang, Teck Kwang Choo</i>	
Statistical Evaluation of Mineral Carbonation of a Fly Ash/Brine System.....	24
<i>Grace Muriithi, Leslie F. Petrik, Wilson M. Gitari, Frédéric J. Doucet</i>	
Ex situ CO₂ Mineralization Using Reactive Species.....	25
<i>Juan Ma, Roe-Hoan Yoon</i>	

Base Metal Production From CO₂ Capture and Storage Via the Ics Integrated Mineral Carbonation Process	30
<i>Richard Hunwick</i>	
Coupling Industrial Carbon Mineralisation and Ocean Alkalinity Enhancement.....	31
<i>Phil Renforth, Tim Kruger</i>	
Evaluating the Viability of CO₂ Mineralization Via Reaction of Caustic Waste Materials.....	33
<i>Robert Dilmore, D. Allen, S. W. Hedges, Yee Soong</i>	
The NETL Aqueous Process: History and Recent Developments.....	34
<i>William O'Connor, G. E. Rush, Circe Verba</i>	
Summary Results of Epri's Engineering and Economic Case Studies of Post Combustion Capture Retrofit Applied to Various North American Host Sites	35
<i>Des Dillon</i>	
Electrochemical Membrane for Carbon Dioxide Separation and Power Generation.....	37
<i>Stephen Jolly, Hossein Ghezel-Ayagh, Jennifer Hunt, Dilip Patel, William A. Steen, Carl F. Richardson, Olga A. Marina</i>	
Modeling, Simulation and Optimization of Absorption, Membrane and Adsorption-Based CO₂ Capture for Variable Feed CO₂ Concentration and Feed Flow.....	44
<i>M. M. Faruque Hasan, Richard C. Baliban, Josephine A. Elia, Christodoulos A. Floudas</i>	
Pressure Swing Adsorption: Design and Optimization for Pre-Combustion Carbon Capture.....	45
<i>Alexander W. Dowling, Lorenz T. Biegler, David C. Miller</i>	
Assessment and Analysis of Post-Combustion Carbon Capture with Membrane Separation Technology	46
<i>Xiangping Zhang, Xuezhong He, Truls Gundersen</i>	
Dynamic Modelling and Analysis of Post-Combustion CO₂ Capture Processes	49
<i>Niall Mac Dowell, Nilay Shah</i>	
Comparisons of Solvents for Post-Combustion CO₂ Capture Using a Multi-Objective Analysis Approach	50
<i>Anita S. Lee, John R. Kitchen</i>	
Post-Combustion Gas Permeation Carbon Capture System Models	51
<i>Juan E. Morinelly, David C. Miller</i>	
Fuel Processing: Renaissance of the Second Decade (Keynote)	52
<i>Brant A. Peppley, Rajesh D. Parmar, Kunal Karan</i>	
Desulfurization of JP-8 Fuel Using Ag-Loaded Silica Supports Under Ambient Conditions	55
<i>Dat T. Tran, Jessica St. John, Deryn Chu, Scott R. J. Oliver</i>	
Desulfurization of Commercial Fuels Using Mixed Oxide Supported Silver Adsorbents At Room Temperature for Fuel Cell Applications	56
<i>A. H. M. Shahadat Hussain, Hongyun Yang, Bruce J. Tatarchuk</i>	
Multi-Physics Modeling of Auto-Thermal Diesel Surrogate Reforming.....	57
<i>Rajesh D. Parmar, Amrit Jalan, Dushyant Shekhawat, William H. Green Jr., Brant A. Peppley, Kunal Karan</i>	
Heat-Integrated Steam Reformer for Hydrogen Production.....	58
<i>Saurabh A. Vilekar, Christian Junaedi, Kyle Hawley, Dennis Walsh, Subir Roychoudhury</i>	
Diesel Reforming Over Pyrochlore-Based Monolith	59
<i>Daniel J. Haynes, David Berry, Dushyant Shekhawat, Mark W. Smith, Matthew M. Seabaugh, Richard Long, James J. Spivey</i>	
Carbon Deposition Over Supported Rh-Ni Catalysts in Steam Reforming of Liquid Hydrocarbon Fuel for H₂ Production: Influence of Support, Temperature, and Sulfur.....	60
<i>Chao Xie, Yongsheng Chen, Chunshan Song</i>	
Fuel Processing with Diesel Fuel and Kerosene for APU Applications.....	61
<i>Joachim Pasel, Jan Meißner, Remzi Can Samsun, Ralf Peters, Detlef Stolten</i>	
Reactor Design for Diesel Reforming Using a Graded-Composition Monolith.....	68
<i>Mark W. Smith, David A. Berry, Dushyant Shekhawat, Daniel J. Haynes, James J. Spivey, John Zondlo</i>	
Carbon Molecular Sieve Membranes for N₂/CH₄ Separation.....	69
<i>Xue Ning, William J. Koros</i>	
High Performance Carbon Molecular Sieves (CMS) Hollow Fiber Membranes for Natural Gas Separation	70
<i>Nitesh Bhuwania, William J. Koros</i>	
Evaluation of Facilitated Transport Membrane for Olefin/Paraffin Separation	71
<i>Majid Keyvani, Glenn Towe, Ali Hamza</i>	
Gas Transport of Paraffins and Olefins in Liquid Crystal Membranes	86
<i>Feras Rabie, Stephen M. Martin</i>	

Synthesis and Characterization of ZIF-8 Membrane with Exceptionally High Propylene / Propane Separation Performance.....	87
<i>Hyuk Taek Kwon, Sagar Lonkar, Hae-Kwon Jeong</i>	
Design of ZIF/Polyimide Mixed Matrix Membrane for Olefin/Paraffin Separations.....	89
<i>Chen Zhang, William J. Koros</i>	
TR Polymers for Olefin/Paraffin Separation.....	90
<i>Zachary P. Smith, David F. Sanders, Ruilan Guo, Benny Freeman, Donald R. Paul, James E. McGrath</i>	
Asymmetric Hollow Fiber Membranes for Aggressive Sour Gas Purification.....	91
<i>Brian E. Kraftschik, William J. Koros</i>	
Carbonate Ceramics and Concrete: A Disruptive Technology for CO₂ Utilization and the Construction Business	92
<i>Richard Riman, S. Gupta, Q. Li, V. Atakan, Ç. Vakifahmetoglu, J. Azurdia, J. Krishnan, M. A. Bitteto, L. Tang, J. Czerepinski, Larry E. McCandlish, Nick Decristofaro</i>	
Synthesis of CaSiO₃ for Use As a Cementitious Material for Carbonate Concrete	93
<i>Nick Decristofaro, V. Atakan, C. Vakifahmetoglu, L. McCandlish, J. Krishnan, L. Tang, Q. Li, R. E. Riman</i>	
CO₂ Utilization in Concrete Block Production.....	94
<i>Yixin Shao, Liang Hu, Hilal El-Hassan</i>	
Catalyzed Activation of CO₂ by Lewis Base Site in Hybrid Metal Organic Frameworks	97
<i>Liang Chen</i>	
Utilization Technologies for CO₂ Derived From North Dakota Lignite.....	98
<i>Jason D. Laumb, Melanie D. Jensen, Robert M. Cowan, Alexander Azenkeng, Loreal V. Heebink, Laura J. Raymond, Peter A. Letvin</i>	
Harnessing Applied Potential for Sunlight Driven CO₂ Utilization	108
<i>Benjamin R. Buckley</i>	
Accelerating Progress Toward Operational Excellence of Fossil Energy Plants with CO₂ Capture	109
<i>Stephen E. Zitney, Eric A. Liese, Priyadarshi Mahapatra, Richard Turton, Debangsu Bhattacharyya</i>	
Characterization and CO₂ Sorption Properties of Materials for CCS Applications.....	164
<i>Jiajun He, Erik C. Rupp, Jennifer Wilcox</i>	
Reducing Uncertainties in Model Predictions Via History Matching of CO₂ Plume Migration At the Sleipner Project, Norwegian North Sea	165
<i>Peng Lu, Chen Zhu, Per Aaggard</i>	
Gas Hydrates Modeling: Spanning Multiple Scales.....	166
<i>Nagasree Garapati, Srinath Velaga, Brian Anderson</i>	
High-Resolution Numerical Simulation of CO₂ Migration in Saline Aquifers	167
<i>Ruslan Iskhakov, Denis Voskov, Hamdi Tchelepi</i>	
Pore Scale CO₂ Displacement in Sandstone with Comparison to Core Scale Dynamics	168
<i>Dustin Crandall, Robert P. Warzinski, William O'Connor, Aslam M. Kabir, Grant Bromhal</i>	
Modeling of Pressure and Displacement Signatures for Detecting A Fracture in the Caprock During Geologic Sequestration	169
<i>Hema Siriwardane, Raj Gondle, Grant Bromhal</i>	
Effect of Calcite Dissolution On the Leakage Through Abandoned Wells in Geological CO₂ Storage	172
<i>Ezzeddine Laabidi, Rachida Bouhlila</i>	
Hydrogen Production From Glycerol Reforming Over Hydrogen Production From Glycerol Reforming Over Ni Based Catalysts.....	173
<i>Dong-Ju Moon, Su Hyun Cho, Seung-Hoon Kim, Seung-Hwan Lee, Bang Hee Kim, Sang Woo Kim, Arunabha Datta, Kwan-Young Lee</i>	
Computer Simulation of Water and Ammonia Electrolysis.....	175
<i>Ali Estejab, Damilola A. Daramola, Gerardine G. Botte</i>	
Desulfurization of JP-8 Fuel Using Metal-Loaded Meso/Macroporous Aluminosilicates	177
<i>Jessica St. John, Dat T. Tran, Deryn Chu, Scott R. J. Oliver</i>	
A Novel KMgAl Sorbent for CO₂ Capture in a Fluidized Bed	178
<i>Fukui Xiao, Wei Wei, Lei Li, Xia Wen, Feng Wang, Ning Zhao</i>	
Microscopic Behavior of Chemical Demulsifiers At the Water-in-Brazilian Asphaltene Model Oil Emulsions: Langmuir Monolayers and Their Corresponding Langmuir-Blodgett Films.....	182
<i>Juliana S. A. Carneiro, Montserrat Fortuny, Alexandre F. Santos, Cláudio Dariva, Elton Franceschi, Bianca M. S. Ferreira, Sandro R. P. Da Rocha</i>	
New Reservoir Opportunities for CCUS: The Bio-Geochemistry of Mobile Water Intervals with Residual Oil: A Permian Basin Case History	183
<i>David Vance, Steve Melzer, Robert Trentham</i>	
Evolution of Carbonate Dissolution Features Produced Under Variable pCO₂ Conditions Relevant to CO₂-EOR and Geologic CO₂ Storage.....	185
<i>Susan Carroll, Megan Smith, Yue Hao</i>	

Opportunities for Utilizing Anthropogenic CO₂ for Enhanced Oil Recovery (EOR)	186
<i>Michael L. Godec</i>	
Potential for CO₂ Enhanced Oil Recovery in the Appalachian Basin	187
<i>Timothy Carr</i>	
Carbon Dioxide Pipeline Infrastructure Dependence On Reservoir Risk	188
<i>Jeffrey Bielicki, Richard Middleton, Melisa Pollak, Elizabeth Wilson, Jeffrey Fitts, Catherine Peters</i>	
A Phased Approach to Developing A Pipeline Network for CO₂ Transport During CCUS	190
<i>Melanie D. Jensen, Peng Pei, Anthony C. Snyder, Loreal V. Heebink</i>	
Micro-Channel Fuel Processors As Hydrogen Source for Fuel Cells in Distributed Energy Supply Systems (Keynote)	196
<i>Gunther Kolb, S. Keller, M. O'Connell, Jochen Schuerer, David Tiemann, Martin Wichert</i>	
Tri-Generation of Hydrogen, Heat and Power From a High Temperature Fuel Cell	198
<i>Jack Brouwer, Roxana Bekemohammadi, Pere Margalef</i>	
Effect of Storage Time On the Catalytic Activity of Gold for Selective CO Oxidation	201
<i>Fabio B. Passos, Thiago S. Mozer</i>	
Hydrogen and Methane Rich Syngas From a Catalytic Coal Gasifier with in Situ Capture of H₂S/CO₂ and Ex Situ Regeneration of Catalysts	202
<i>Nicholas Siefert, Dushyant Shekhawat, Shawn Litster, David Berry</i>	
Molten Salt Gasification (MSG) of Refinery Wastes to Produce Hydrogen	207
<i>Lyman Frost</i>	
Highly Efficient Integrated Chemical Looping Gasification Fuel Cell System	208
<i>Liang Zeng, Mandar Kathe, Siwei Luo, Fanxing Li, Liang-Shih Fan</i>	
Experimental Investigation On the Effects of Trace Contaminants in Coal Derived Syngas On Performance of SOFC Ni-YSZ Anode	209
<i>Koji Kuramoto</i>	
A Microchannel Water-Gas Shift Reactor Simulation and Optimization for a Mobile Application	219
<i>M. H. Akbari, S. A. Asaee</i>	
Microplasma Reforming for Fuel Cell Feed	236
<i>Peter J. Lindner, R. S. Besser</i>	
Dry Reforming Assisted Nonthermal Plasma Catalytic Reactor	243
<i>Mahammadunnisa Shaik, P. Manoj Kumar Reddy, B. Ramaraju, Ch. Surbahmanyam</i>	
Dry (CO₂) Reforming of Methane Using Rh Substituted Pyrochlores (La₂Zr₂O₇)	244
<i>Devendra Pakhare, Victor Abdelsayed, Daniel J. Haynes, Dushyant Shekhawat, James J. Spivey</i>	
Simulation of Methane Steam Reforming Enhanced by in Situ CO₂ Sorption Utilizing K₂CO₃ Promoted Hydrotalcites for H₂ Production	262
<i>Naruewan Chanburanasiri, Ana M. Ribeiro, Alirio E. Rodrigues, Navadol Laosiripojana, Suttichai Assabumrungrat</i>	
Bi-Reforming of Methane and Natural Gas Under High Pressure	270
<i>Alain Goeppert, Miklos Czaun, Robert May, Surya Prakash, George Olah</i>	
Production of Hydrogen and Nanocarbon From Catalytic Decomposition of Methane Over a Ni-Fe/Al₂O₃ Catalyst	272
<i>Yi Jin, Gaowei Wang, Yongdan Li</i>	
Natural Gas Direct Carbon Fuel Cell for Hydrogen and Electricity Production (NGDCFC)	273
<i>Meyer Steinberg</i>	
CFD Simulation of Pressurized, Staged Oxyfuel Combustion	274
<i>Benjamin M. Kumfer, Fei Xia, Bhupesh Dhungel, Richard L. Axelbaum</i>	
Double Perovskite Materials for Applications in Chemical Looping and Oxygen Storage	276
<i>Jonathan W. Lekse, Sittichai Natesakhawat, John P. Baltrus, Christopher Matranga</i>	
Using Ca_xLa_{1-x}Mn_{1-y}M'_yO_{3-δ} As Oxygen Carriers for Chemical-Looping Combustion	277
<i>Tobias Mattisson, Ali Hedayati, Abdul-Majeed Azad, Magnus Ryden, Henrik Leion</i>	
Mechanism of Methane Chemical Looping Combustion with Fe₂O₃ Promoted with CeO₂	285
<i>Duane Miller, Ranjani V. Siriwardane</i>	
Oxygen Carriers for Chemical-Looping Combustion with Solid Fuels	286
<i>Tobias Mattisson, Henrik Leion, Magnus Ryden, Anders Lyngfelt</i>	
Development and Performance Evaluation of a Cost-Effective Oxygen Carriers	294
<i>Liangyong Chen, Yi Zhang, Fang Liu, Chunli Han, James K. Neathery, Kunlei Liu</i>	
Study of Wyoming PRB Coal for Application of Solid Fueled Chemical Looping Combustion with TGA-MS	295
<i>Yi Zhang, Jeffrey Slone, Aurora M. Rubel, James K. Neathery, Fang Liu, Chunli Han, Liangyong Chen, Kunlei Liu</i>	
Techno-Economic Evaluation of Chemical Looping Combustion for Industrial-Scale Applications	296
<i>John T. Ramsey, Michael J Gallagher Jr., Stephen Carpenter, George Richards</i>	

CFD Modeling of Commercial-Scale Entrained-Flow Coal Gasifiers	297
<i>Jinliang Ma, Stephen E. Zitney</i>	
Ultrasound Measurements of Temperature Profile Across Gasifier Refractories	298
<i>Yunlu Jia, Mikhail Skliar</i>	
Recent Developments in Carbonaceous Chemistry for Computational Modeling (C3M) with Uncertainty Quantifications (UQ)	302
<i>Kiran Chaudhari, Richard Turton, Chris Guenther, Mehrdad Shahn timer, Aytekin Gel, Philip Niccolleti, Tingwen Li, Dirk Vanessendelft, Nate Weiland</i>	
A One-Dimensional Transient Model of a Single-Stage, Downward-Firing, Entrained-Flow Gasifier	303
<i>Job Kasule, Richard Turton, Debansu Bhattacharyya, Stephen E. Zitney</i>	
Co-Pyrolysis of Low Rank Coals and Biomass At Transport Gasifier Conditions	304
<i>Nathan T. Weiland, Nicholas C. Means, Chris Guenther</i>	
Dynamic Modeling of Detachment, Transport, and Flow of Slag in an Entrained-Flow Gasifier	311
<i>Pratik Pednekar, Debansu Bhattacharyya, Richard Turton, Raghunathan Rengaswamy</i>	
Hydrogen Production From Renewable Sources: R&D Challenges, Targets and Pathways (Keynote)	313
<i>Sara Dillich, Eric Miller, Erika Sutherland, Sarah Studer</i>	
Auto-Thermal Reforming of Biodiesel-Ethanol-Diesel Blends for Solid Oxide Fuel Cell Applications	315
<i>Jiefeng Lin, Thomas Trabold, Mark Walluk, Daniel Smith</i>	
Development of a Butanol Fuel Processor for Person-Portable Fuel Cell Power Systems	323
<i>Stephen Jolly, Hossein Ghezel-Ayagh</i>	
Cartridge-Based Ceramic Microreactor Networks for Process Intensification in Fuels Reforming: Demonstration and Modeling of Complex 2-D Thermal Integration	324
<i>Bhanu Vardhan Reddy Kuncharam, Shalini Damodharan, Benjamin Wilhite</i>	
Protonic Membrane Reactors: Converting Hydrocarbon Resources and CO₂ to Fuels	325
<i>Eric D. Wachsman</i>	
One-Stage Process for Water Gas Shift in a Pd-Based Membrane Reactor	326
<i>Giuseppe Barbieri, Adele Brunetti, Alessio Caravella, Enrico Drioli</i>	
Water Gas Shift Reaction in Thin Pd-Layer Supported On PSS Membrane Reactor	328
<i>Angelo Basile, Pietro Pinacci, Francesca Drago, Simona Liguori, Pietro Paolo Morrone, Adolfo Iulianelli</i>	
Techno-Economic Assessment of Membrane Reactor Technologies for Pure Hydrogen Production for Fuel Cell Vehicle Fleets	329
<i>Leonardo Roses, Giampaolo Manzolini, Stefano Campanari, Ellart De Wit, Michael Walter</i>	
Experimental and Simulation Studies of Effects of Operating Conditions and Membrane Properties On the Performance of Zeolite Membrane Reactors for High Temperature Water Gas Shift Reaction	345
<i>Seok-Jhin Kim, Shaowei Yang, Junhang Dong</i>	
Pore Scale Models for Imbibition of CO₂ Analogue Fluids in Etched Micro-Model Junctions Using Micro-Fluidic Experiments and Direct Flow Calculations	346
<i>Emily Chapman, Jianhui Yang, John Crawshaw, Edo Boek</i>	
Selection of Domain Size for Lattice Boltzmann Simulation to Calculate Flow Properties of Porous Media	347
<i>Md Rakibul Sarker, Shameem Siddiqui, Dustin McIntyre, Grant Bromhal, Mohamed Soliman</i>	
A Lattice Boltzmann Model with Realistic Equations of State for Modeling Pore-Scale Effects On Capillary Trapping of CO₂ During Geological Carbon Sequestration	348
<i>Marcel Schaap, Dorte Wildenschild</i>	
Insights From Image-Based Modeling of Fluid Flow in Bulk Proppant Packs and Propped Fractures Under Varying Confining Stress	350
<i>Yijie Shen, Paula Sanematsu, Seth M. Bradley, Clinton S. Willson, Ali Takbiri Borujeni, Karsten E Thompson, Mayank Tyagi</i>	
Recent Trends of Streamline Simulation Technology Applications in Oil Industry	351
<i>Abdullah Al-Najem, Shameem Siddiqui, Mohamed Soliman</i>	
Hydrogeochemical Modelling in Coastal Carbonate Aquifer: Porosity and Permeability Evolution	366
<i>Rachida Bouhlila, Ezzeddine Laabidi</i>	
Structure Sensitivity of Methanol Synthesis From Carbon Dioxide On Copper-Based Catalysts	377
<i>Sittichai Natesakhawat, Victor Abdelsayed, Jonathan W. Lekse, John P. Baltrus, Paul R. Ohodnicki Jr., Bret H. Howard, Xingyi Deng, Christopher Matranga</i>	
Fluorine-Modified Cu/Zn/Al/Zr Catalysts Via Hydrotalcite-Like Precursors for the CO₂ Hydrogenation to Methanol	378
<i>Fukui Xiao, Peng Gao, Li Feng, Ning Zhao, Wei Wei, Yuhan Sun</i>	
Dehydrogenation of Ethylbenzene to Styrene with CO₂ Over V₂O₅/Al₂O₃-ZrO₂ Catalyst	385
<i>Shujiao Zhang, Xiaohong Li, Jie Feng, Wenying Li, Hongxia Fan, Qian Wang</i>	

A Comparative Study of Activated CO₂ Adsorption and Protonation On the γ-Al₂O₃, β-Ga₂O₃, In₂O₃ Surfaces	397
<i>Jingyun Ye, Changjun Liu, Qingfeng Ge</i>	
C-H Activating Carboxylation of Terminal Alkynes with CO₂ and Its Application in Synthesis	398
<i>Yugen Zhang, Jackie Y. Ying, Dingyi Yu, Siti Riduan</i>	
Photochemical Reduction of CO₂ Using Delafossite Oxides	400
<i>Jonathan W. Lekse, James P. Lewis, M. Kylee Underwood, Christopher Matranga</i>	
Two-Step Solar Thermochemical Cycle for Splitting CO₂ Via Ceria Redox Reactions - Experimental Investigation with a 3.8 Kw Solar Reactor	401
<i>Philipp Furler, Jonathan Scheffe, Aldo Steinfeld</i>	
Applicability of Perovskite-Based Oxides As Redox Materials for Thermochemical CO₂ Dissociation	402
<i>Jonathan Scheffe, David Weibel, Aldo Steinfeld</i>	
Bench-Scale Electrochemical Production of Synthesis Gas	403
<i>Eric Dufek, Tedd Lister, Michael McIlwain</i>	
Electrode and Catalyst Design for Electrochemical Reduction of CO₂	411
<i>Molly Jhong, Sichao Ma, Paul J. A. Kenis</i>	
CO₂ - Ionic Liquids Synergies: Reactive Capture and Conversion of CO₂ to Chemicals	413
<i>Valerie Eta, Pasi Virtanen, Ikenna Anugwom, Päivi Mäki-Arvela, Jyri-Pekka Mikkola</i>	
Numerical Simulation of Reservoir-Wellbore Fluid Flow Simulations At Geologic CO₂ Sequestration Sites: Coupled or De-Coupled?	415
<i>Rajesh Pawar, Haruko Wainwright, Robert Dilmore, Jens Birkholzer, Jim Houseworth, Grant Bromhal</i>	
Investigating the Role of Coupled Thermal-Hydrological-Mechanical (THM) Processes During Geological Sequestration of CO₂	416
<i>Sharad Kelkar, Rajesh Pawar, George A. Zyvoloski, Philip Stauffer, Hari Viswanathan</i>	
Reservoir Model Optimization Using the Seismic Response to CO₂ Injection and Stochastic Inversion	417
<i>Abelardo Ramirez, Kathy Dyer, Donald J. White, Yue Hao, James Johnson</i>	
Assessing the Role of Thermal Stresses in Caprock Integrity During CO₂ Storage	418
<i>Gennady Gor, Jean-Herve Prevost</i>	
Cement Degradation Under Conditions Relevant to Geological Carbon Sequestration	419
<i>Leopold Brunet, Li Li, Zuleima Karpyn, Brian Strazisar, Barbara Kutchko</i>	
Laboratory and Numerical Simulation Based Investigation of Two-Phase Brine-CO₂ Displacement Processes Using Cores From Three CO₂-Sequestration Candidate Formations	426
<i>Shameem Siddiqui, Talal Gamadi, Otman Algadi, Abdulrahman A. Alquraishi, Dustin McIntyre</i>	
Modification of Fracture Hydraulic Properties by CO₂-Acidified Brine Flow	437
<i>Hang Deng, Brian R. Ellis, Catherine Peters</i>	
New Experimental Data and Physico-Chemical Model for the Solubility of Carbon Dioxide in Aqueous Solutions of Monoethanolamine	438
<i>Michael Wagner, Inga Von Harbou, Jaeik Kim, Gerd Maurer, Hans Hasse</i>	
Mass Transfer Evaluation of CO₂ Absorption in a Wetted Wall Column	439
<i>Reynolds A. Frimpong, Joseph E. Remias, James K. Neathery, Kunlei Liu</i>	
Kinetic Study of Carbon Dioxide Absorption by Aqueous Solutions of N-Methyldiethanolamine and Piperazine	440
<i>Alberto Servia, Nicolas Laloue, Julien Grandjean, Sabine Rode, Christine Roizard</i>	
Aqueous Morpholine As a Potential Post-Combustion CO₂ Absorption Solution	446
<i>Krishna Mohan Jinka, Taylor Kuhn, Joseph E. Remias, James K. Neathery, Kunlei Liu</i>	
Novel Liquid-Like Nanoscale Organic Hybrid Materials for CO₂ Capture	447
<i>Camille Petit, Youngjune Park, Kunyi Andrew Lin, Ah-Hyung Alissa Park</i>	
Development of Reaxff Force Field for Carbon Dioxide Capture with Ionic Liquids: A Combined First Principles and Classical Simulation	448
<i>Bo Zhang, Adri C. T. Van Duin, Karl Johnson</i>	
Vibrational Spectroscopy Characterization of CO₂-Ionic Liquid Systems for Pre-Combustion CO₂	449
<i>Anita S. Lee, John R. Kitchin</i>	
Evaluation of Mercury Capture Technology Using Various Sorbents Injection	450
<i>Xiaofei Wang, Pratim Biswas</i>	
Overview on Mercury Control Options for Coal-Burning Power Plants	451
<i>Evan J. Granite, Henry W. Pennline</i>	
Palladium Sorbents for High Temperature Capture of Mercury, Arsenic, Selenium and Phosphorus from Fuel Gas	452
<i>Evan J. Granite, Henry W. Pennline, Erik C. Rupp, Dennis Stanko, John P. Baltrus, Hugh Hamilton, Liz Rowsell, Stephen Poulston, Andrew Smith, Wilson Chu, Tony Wu</i>	
Author Index	