Energy Technology 2015
Carbon Dioxide Management and Other Technologies

Edited by
Animesh Jha
Cong Wang
Neale R. Neelameggham
Donna P. Guillen
Li Li
Cynthia K. Belt
Randolph Kirchain
Jeffrey S. Spangenberg
Frank Johnson
Andrew J. Gomes
Amit Pandey
Peter Hosemann
Energy Technology 2015
Carbon Dioxide Management and Other Technologies
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Energy Technology 2015
Carbon Dioxide Management and Other Technologies

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Additional papers have been contributed by the following symposia:

Recycling and Sustainability Update
Sponsored by the Recycling and Environmental Technologies Committee of EPD and LMD

Magnetic Materials for Energy Applications V
Sponsored by the Magnetic Materials Committee of the TMS Functional Materials Division (FMD, formerly the Electronic, Magnetic & Photonic Materials Division)

Sustainable Energy and Layered Double Hydroxides
Sponsored by the Chemistry and Physics of Materials Committee of FMD and the TMS Structural Materials Division (SMD)

High-Temperature Systems for Energy Conversion and Storage
Sponsored by the Energy Conversion and Storage Committee of FMD

Sponsored by the Corrosion and Environmental Effects Committee and Nuclear Materials Committee of SMD, and the Energy Conversion and Storage Committee of FMD

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TABLE OF CONTENTS
Energy Technology 2015

About the Editors ........................................................................................................... xi
Session Chairs .............................................................................................................. xix

Energy Technologies and Carbon Dioxide Management Symposium 2015

Carbon Management

A Thermodynamic Study of Mixed Carbon Feedstock Gasification Slags ........ 5
J. Nakano, M. Duchesne, J. Bennett, K. Kwong, and A. Nakano

Evaluation of Heat Treatment Performance of Potential Pipe Steels
in CCS-Environment ................................................................................................. 15
A. Pfennig, H. Wolthusen, P. Zastrow, and A. Kranzmann

Economic Assessment of Methanol Synthesis by CO\textsubscript{2} from Coal-Fired
Power Plants ........................................................................................................... 23
Y. Wang and Y. Dai

Thermal Wastes from Energy Conversions and Global Anthropogenic
Warming .................................................................................................................. 29
N. Neelameggham and B. Davis

Iron & Steel

Influence of the Initial Solidification Controlling on the Energy
Saving during Continuous Casting ............................................................................ 39
L. Zhou and W. Wang

Performance of Twin Oxygen-Coal Lances for PCI Operation in
Blast Furnace Iron Making ...................................................................................... 47
F. Meng, H. Tang, and Z. Zhao

Energy Saving and CO\textsubscript{2} Emission Reducing Analysis of Chinese
Iron and Steel Industry ............................................................................................. 55
Q. Zhang, Y. Li, Y. Shen, and H. Dong

Investigation on the Heat Recovery from High Temperature Slags .................. 65
Y. Sun and Z. Zhang
Optimal Distribution of Byproduct Gases in Iron and Steel Industry
Based on Mixed Integer Linear Programming (MILP) .........................................73
   X. Zhao, H. Bai, Q. Shi, J. Han, and H. Li

**Metal Processing / Molten Salt / Electrochemistry**

Energy Efficient Separation of Magnetic Alloy from the Carbothermic Reduction of Nkana Cu-Co Concentrates .................................................................83
   Y. Hara and A. Jha

LCA Evaluation for Different Treatment Processes of Nickel Laterite Ore .........................................................................................................................93
   S. Wang, H. Li, C. Li, X. Hao, Q. Bao, and L. Zhang

Low Temperature Sulphidization of Cu-Co Slag in the Presence of Calcium Sulphide .................................................................................................105
   Y. Hara and A. Jha

A Kinetic Analysis of Acid Leaching of Niobium and Zirconium from Titania Waste Residue Stream: An Energy Efficient Methodology for the Reclamation of Metal Values .........................................................115
   T. Makanyire, A. Jha, and S. Sutcliffe

The Optimization Formula Design of Cu$_x$Zn$_{1-x}$O Infrared Radiation Material and Coating Slurry .............................................................................123
   Y. Ding, H. Bai, C. Lian, W. Wei, and W. Liu

The Role of Austenitizing Routines of Pipe Steels during CCS ..................131
   A. Pfennig, J. Schiz, and A. Kranzmann

Evaluation of Surface Tension for the NaNO$_3$-KNO$_3$-Ca(NO$_3$)$_2$ System and Its Sub-System ..................................................................................139
   J. Xu, J. Zhao, J. Wang, J. Li, and K. Wan

**Solar Energy**

Development of High Flux Solar Simulators for Solar Thermal Research ......149
   B. Ekman, G. Brooks, and M. Rhamdhani

vi
Recycling and Sustainability Update

Waste

The Removal of Phosphate and Ammonia Nitrogen from Wastewater Using Steel Slag ................................................................. 165
  X. Ping, Y. Liyun, R. Aikebaier, and B. Hao

Sustainable Recycling Technologies for Bauxite Residue (Red Mud) Utilization ................................................................. 173
  J. Ahn, T. Thriveni, and S. Nam

Recycling

Investigation on Recycling of Ag from Pb-Cu-Ag Alloy by Vacuum Distillation ................................................................. 183
  B. Song, W. Jiang, B. Yang, B. Xu, Q. Yang, S. Xu, and D. Liu

Recycling of Sinter Plant Offgas Cleaning System Dust by Pre-Agglomeration ................................................................. 193
  N. Ma

Recovery of Metals from Waste Printed Circuit Boards by Leaching with 1-Ethyl-3-Methyl-Imidazolium Hydrogen Sulfate Ionic Liquid ........ 201
  T. Atalay, A. Kilıçarslan, and M. Sarıdede

Application of 1-Methylimidazolium Hydrogen Sulfate Ionic Liquid to the Oxidative Leaching of Copper and Zinc in Industrial Brass Dross .... 209
  A. Kilıçarslan and M. Sarıdede

Poster Session

Experimental Study on Reduction in Low Grade Lateritic Nickel Ore Mixed with Pickling Sludge ..................................................... 219
  Y. Feng, Y. Sun, J. Zhang, and Q. Li

Recycling Wastes in the Alumina and the Cement Industry ........................... 227
  N. Ilyoukha and V. Timofeeva

Evaluation of the Silver Recovery from Radiographic Films in a Filter Press Electrochemical Reactor ........................................ 233
  P. Ortega, V. Cruz, L. Hernández, D. Islas, M. Guerrero, and L. Lechuga
Magnetic Materials for Energy Applications

Soft Magnetic Materials I

Effect of Electric Current Pulse on Grain Boundary of Grain Oriented Silicon Steel during Primary Recrystallization Annealing ............................................255
Z. Lu, L. Li, W. Nan, X. Jiang, and Q. Zhai

Soft Magnetic Materials II

Magnetostriction of Co-Fe-Based Amorphous Soft Magnetic Microwires .....265
A. Zhukov, M. Churyukanova, S. Kaloshkin, V. Sudarchikova,
S. Gudoshnikov, M. Ipatov, A. Talaat, J. Blanco, and V. Zhukova

Poster Session

Magnetostressitional Transition in Heusler Mn-Ni-In Melt Spun Ribbons ........ 275
H. Li, J. Ren, J. Yu, and H. Zheng

Magnetic Properties of Nanocrystalline Microwires .................................283
A. Talaat, V. Zhukova, M. Ipatov, J. Blanco, P. Klein, R. Varga,
L. Gonzalez-Lagarreta, B. Hernando, and A. Zhukov

On Magnetocaloric Properties of (Pr,Dy)Fe₉ Alloys ..............................291
R. Guetari, C. Cizmas, K. Zehani, L. Bessais, and N. Mliki

Sustainable Energy and Layered Double Hydroxides

Technical Innovation and Entrepreneurial Potential of “Hydrotalcite Like” Materials .................................................................301
D. Cocke, P. Latiolais, A. Gomes, and G. Beall

Layered Double Hydroxides in Energy Research: Advantages
and Challenges .................................................................309
   A. Gomes, D. Cocke, D. Tran, and A. Baksi

Modelling the Structure and Vibrational Properties of Layered
Double Hydroxides ................................................................317
   E. Andre, J. Fahel, and C. Carteret

Synthesis of Hydrotalcite-Like Compounds from Blast Furnace Slag:
The Effect of Synthesis Parameters on Structure and Crystallinity ........325
   M. He, J. Zhang, Z. Shi, F. Liu, and X. Li

High-Temperature Systems for Energy Conversion and Storage

Solid Oxide Fuel Cell: Recent Developments II

   Evaluating Electrophoretically Deposited Cu-Mn-O Spinel Coatings on
Stainless Steel Substrates Used in Solid Oxide Fuel Cell Interconnects ....337

Innovation in Energy Conversion and Storage I

   Degradation of Sm$_2$Zr$_2$O$_7$ Thermal Barrier Coating Caused by
Calcium-Magnesium-Aluminum-Silicon Oxide (CMAS) Deposition .........347

Structural Materials, Heat Transport Fluids, and
Novel System Designs for High Power and Process
Heat Generation

Heat Transport Fluids I

   Minimum System Entropy Production for the Figure of Merit of High
Temperature Heat Transfer Fluid Properties .......................................359
   P. Li and Y. Zhang

Author Index ..................................................................................373

Subject Index ..................................................................................375
Animesh Jha

Animesh Jha has been a professor of materials science at the University of Leeds in the United Kingdom since August 2000. He obtained his Bachelor of Engineering (BE) degree in metallurgy in June 1979 from the University of Roorkee (India); his Master of Engineering (ME) degree in metallurgical engineering in July 1981 from the Indian Institute of Science, Bangalore in India; and Ph.D. and DIC from Imperial College (London) in October 1984 in the area of chemical and process metallurgy. After earning his Ph.D., he did a short postdoctoral research engagement at Purdue University (US) in 1985-86, before returning to Sheffield, UK in December 1986 where he started research on phase transformations in novel salt-based and metallic glass systems. In May 1989, he took his academic position at Brunel University, Uxbridge, UK where he developed his academic career in the areas of IR glasses and mineral processing. He has since 1989 continued research in these two areas and produced over 24 Ph.D. theses from 1992 to 2014.

He has published over 400 research papers in peer-reviewed journals and reviewed conference proceedings. He has been a member of TMS since 1992, a fellow of the Institute of Physics in London, and member of the Optical Society of America and IEEE. He serves as an external reviewer for overseas research agencies including US, Canada, and EU countries. He is also actively involved in translational research, which allows the lab work to reach industry.

Cong Wang

Cong Wang is currently a professor of the School of Materials and Metallurgy, Northeastern University. Previously, he held positions at Northwestern University, Saint-Gobain High Performance Materials Research and Development Center, and Alcoa Technical Center. He is a seasoned metallurgist/materials scientist with rich experience in aluminum alloys, copper alloys, iron and steels, magnesium alloys, and super-abrasives. He obtained his Ph.D. from Carnegie Mellon University; M.S. from the Institute of Metal Research, Chinese Academy of Sciences; and B.S. from Northeastern University with distinctions, respectively.

**Neale R. Neelameggham**

Neale R. Neelameggham is ‘The Guru’ at IND LLC, involved in technology marketing and international consulting in the field of light metals and associated chemicals (boron, magnesium, titanium, lithium, and alkali metals), rare earth elements, and battery and energy technologies. He was recently a visiting expert at Beihang University of Aeronautics and Astronautics, Beijing, China. He has over 38 years of expertise in magnesium production and was involved in process development of its startup company NL Magnesium through to the present US Magnesium LLC, UT from where he retired in 2011. He is developing thiometallurgical processes – a new concept of using sulfur as the reductant and or fuel. He has published a heat transfer model for global anthropogenic warming based on thermal emissions independent of energy conversion source.

Dr. Neelameggham holds 16 patents and patent applications, and has published several technical papers. He has served in the Magnesium Committee of the TMS Light Metals Division (LMD) since its inception in 2000, chaired it in 2005, and in 2007 he was made a permanent co-organizer for the Magnesium Technology Symposium. He has been a member of the Reactive Metals Committee, Recycling Committee, and Titanium Committee; and a Programming Committee Representative of LMD. In 2008, Dr. Neelameggham was the inaugural chair of the Energy Committee, a joint committee between the TMS Light Metals and Extraction and Processing Divisions, and has been a co-editor of the Energy Technology symposium through the present. He received the LMD Distinguished Service Award in 2010. He is the Chairman of Hydrometallurgy and Electrometallurgy Committee of the Extraction and Processing Division for the 2013-2015 term, during which time he organized the Rare Metal Technology 2014 and 2015 symposia. He is the co-editor for the *Essential Readings in Magnesium Technology* compendium of TMS papers published in 2014. He is a co-editor of 2015 symposium on *Drying, Roasting and Calcining*. 

xii
Donna P. Guillen
Donna Post Guillen is a Distinguished Staff Engineer and Group Lead in the Advanced Process & Decision Systems Department at the Idaho National Laboratory (INL). Dr. Guillen earned a B.S. in Mechanical Engineering from Rutgers University, an M.S. in Aeronautics from Caltech, and a Ph.D. in Engineering and Applied Science from Idaho State University. She is a registered Professional Engineer in Mechanical Engineering in the State of Idaho. She has served as Principal Investigator for several multidisciplinary research projects on the topics of waste heat recovery, synthetic fuels production, nuclear reactor fuels and materials experiments, and waste glass processing. The focus of her research is on multiphase computational fluid dynamics (CFD) and thermal hydraulics for sustainable energy technologies. She applies numerical modeling techniques to provide understanding of a wide variety of complex systems, from greenhouse gas generation/sequestration for dairies to waste vitrification for the Hanford Waste Treatment Plant. Dr. Guillen is especially interested in materials as they relate to heat transfer and fluid flow phenomena. She is experienced with irradiation testing and thermal hydraulic analysis for ATR experiments and serves as Principal Investigator / Technical Lead for the ATR National Scientific User Facility (NSUF) Program. She is the lead inventor on two patents related to the development of a new composite material to produce a fast reactor environment within a pressurized water reactor, such as ATR. She actively mentors students; routinely chairs and organizes technical meetings for professional societies; serves in leadership capacity for the American Nuclear Society (Thermal Hydraulics Executive and Program Committees), The Minerals, Metals & Materials Society (Energy Committee Chair), and the American Society of Mechanical Engineers (Thermal Hydraulics and CFD Studies Track Chair); provides subject matter reviews for proposals and technical manuscripts; has published over 100 conference papers, reports, and journal articles; and has written/edited three books.

Li Li
Li Li is a Senior Research Associate in Department of Materials Science and Engineering of Cornell University. He received his Ph.D. degree in Materials Science and Engineering from Carnegie Mellon University (CMU) in 2012; two master degrees from CMU and Harbin Institute of Technology (HIT); and bachelor degree from HIT, respectively. Dr. Li is a talented materials scientist with expertise in energy materials processing, solar energy conversion, and energy storage. He has authored more than
30 technical journal papers and is the reviewer of more than 30 prestigious journals, including *Energy & Environmental Science* and *Metallurgical and Materials Transactions*. He has frequently chaired symposia at TMS and MRS Annual Meetings and is the member of TMS Energy Committee. Because of his contribution to the materials science, he has been awarded to represent TMS at the Emerging Leaders Alliance Conference in 2014.

**Cynthia K. Belt**

Cindy Belt has managed energy programs at Superior Industries, Aleris International, and Kaiser Aluminum. She has published multiple papers in the area of energy management in the metals industry and has co-edited several proceedings in energy and recycling.

Cindy is Vice-Chair of the TMS Extraction and Processing Division, Past-Chair of the Energy Committee, and a member of Materials and Society committee within TMS and is involved in numerous energy groups within TMS, AFS, and ASME. Cindy earned her Bachelor of Science in Mechanical Engineering degree from Ohio Northern University.

**Recycling and Sustainability Update**

**Randolph Kirchain**

Randolph Kirchain’s research and teaching aim to improve materials-technology decisions by characterizing the economic and environmental impact of those decisions. That impact may derive from changes in the performance of the products into which those materials are transformed and/or in the systems in which they are produced, used, and eventually discarded. Dr. Kirchain has authored over 100 publications in refereed journals and conferences. He has been awarded the American Iron and Steel Institute’s Top Technical Achievement Award, the General Motors Technical Achievement Award, and the TMS Recycling Technology Award. Currently, Dr. Kirchain serves as the co-director of the MIT Concrete Sustainability Hub.
Jeffrey S. Spangenberger
Jeffrey Spangenberger is a senior engineering specialist at Argonne National Laboratory with a B.S. in chemical engineering from Iowa State University. Working in the Energy Systems Division’s Process Technology Group, Jeff has lead research activities ranging in scale from bench top testing through full scale plant installations and process efficiency studies. While he works to find ways of reducing energy demands in many energy intensive processes, much of his work relates to the separation and recovery of materials in waste streams destined for landfill. This research has resulted in the conceptualization, design, and construction of equipment, pilot scale processes and industrial scale plants resulting in numerous patents and awards.

Magnetic Materials for Energy Applications V

Frank Johnson
Frank Johnson joined GE Global Research in 2005 as a materials scientist in ceramic and metallurgy technologies. His current research focuses on the development of magnetic materials for power generation, distribution, and conversion technologies. Frank’s area of expertise is the structure-processing-property relationships of crystalline, nanocrystalline, and amorphous soft magnetic alloys, rare-earth permanent magnets, and magnetocaloric materials. Prior to joining GE, Frank received was a post-doctoral fellow in the Magnetic Materials Group, Metallurgy Division of the National Institute of Standards and Technology in Gaithersburg, Maryland. While at NIST, he worked on magnetocaloric materials, magnetic thin-films, and assisted in the development of magnetic standard reference materials. Dr. Johnson received his Ph.D. in materials science and engineering from Carnegie Mellon University in 2003, and his thesis topic was in the area of Fe-Co based nanocrystalline soft magnetic alloys (HITPERM). He received an M.S. in materials science and engineering from the Massachusetts Institute of Technology in 1999 and a B.S. in materials science and engineering from Carnegie Mellon University in 1996.
Sustainable Energy and Layered Double Hydroxides

Andrew Jewel Gomes
Andrew Jewel Gomes received his doctoral degree in Physical Chemistry from Bergische Universitaet Wuppertal, Germany in 2002. He is currently employed as Research Associate Professor in the College of Engineering at Lamar University in Beaumont, Texas. He has been involved in research for more than two decades in a variety of areas, such as waste water treatment, electrochemistry, air pollution remediation, materials synthesis and characterization, and Gaussian simulation. His number of publication is 70 including 24 peer-reviewed articles. He is co-author of Yaws Handbook, and has contributed as chapter author in the book titled Hazardous Materials: Types, Risks and Control. His research group is currently involved in developing NOx and SOx removal device using layered double hydroxides in combustion system.

High-Temperature Systems for Energy Conversion and Storage

Amit Pandey
Amit Pandey’s career has been multidisciplinary and he has worked in industry, academics, and national laboratory of higher research and education. Currently he is working as a development lead in reliability at Rolls Royce LG Fuel Cell Systems, Inc., in Ohio. He started working in the field of thermal barrier coatings at Johns Hopkins University as a postdoctoral fellow in the department of mechanical engineering. Later he was awarded the research fellowship at the Oak Ridge National Laboratory in the Materials Science and Technology Division. During his time at ORNL he developed new characterization techniques to study the thermomechanical response of porous and microcracked ceramics systems (Cordierite for filtration, active layers in the solid oxide fuel cells, coatings for turbine blades, etc.).

In the short span of his professional career Dr. Pandey has published aggressively and has received various awards showing his academic excellence and exemplary leadership ability. This includes the recent 2014 TMS Young Professional Award from TMS Functional Materials Division (formerly the Electronic, Magnetic, and Photonic Materials Division) and 2014 American Ceramic Society’s Future Leader. He has also been involved as an organizing chair and co-chair of symposia for high
temperature materials in particular in the area of functional ceramics for energy conversion and storage.

Dr. Pandey also serves as a director on the executive committee of ASME and ASM International’s Akron, Ohio Chapter. The primary focus of these activities is to increase the interest of students toward the STEM field. Dr. Pandey earned his B.S. in 2003 in mining engineering (rock mechanics) from Indian Institute of Technology (IIT), India. He later received his Master’s degree in 2005 in civil engineering (geomechanics) from University of Arizona and his Ph.D. in 2009 from mechanical engineering (mechanics and materials) from University of Maryland.


**Peter Hosemann**

Peter Hosemann is Associate Professor at the University of California Berkeley in the department of Nuclear Engineering. He joined UCB in 2010 and is responsible for the nuclear materials group. The research focus is on materials in nuclear and other extreme environments with a specific focus on structural materials degradation. Prior to this appointment he was post doctorate associate at Los Alamos National Laboratory from 2008-2010. He graduated from the Montanuniveristaet Leoben in Austria in 2008 from the department of chemistry after receiving his M.S. from the same institution in the department of physics.

Dr. Hosemann is also advisor to the editorial board for the *Journal of Nuclear Materials* while being elected the “best reviewer” for this journal. In addition he serves as key reader and guest editor on other journals. He is a frequent organizer of a number of workshops and symposia including but not limited to several TMS and MRS symposia.
SESSION CHAIRS

Energy Technologies and Carbon Dioxide Management Symposium
2015

Carbon Management
Animesh Jha, University of Leeds
Cynthia K. Belt, Consultant

Iron & Steel
Cong Wang, Northeastern University
Zuotai Zhang, Peking University

Metal Processing / Molten Salt / Electrochemistry
Animesh Jha, University of Leeds
Donna P. Guillen, Idaho National Laboratory
Li Li, Cornell University
Shulan Wang, Northeastern University

Solar Energy
Li Li, Cornell University
Shulan Wang, Northeastern University

Recycling and Sustainability Update
Waste
Jeffrey S. Spangenberger, Argonne National Laboratory

Recycling
Randolph Kirchain, Massachusetts Institute of Technology

Magnetic Materials for Energy Applications V
Magnetocaloric Materials I
Frank Johnson, GE Global Research
Victorino Franco, University of Seville

Permanent Magnets I
Raju Ramanujan, Nanyang Technological University
Ivan Skorvanek, Institute of Experimental Physics
Magnetic Materials for Energy Applications Poster Session
Huseyin Ucar, Oak Ridge National Laboratory
Xiujuan Jiang, Pacific Northwest National Laboratory

Permanent Magnets II
Hariharan Srikanth, University of South Florida
Lin Zhou, Ames Laboratory

Magnetocaloric Materials II
Karl Sandeman, Imperial College of London
Alex Leary, Carnegie Mellon University

Soft Magnetic Materials I
Paul Ohodnicki, National Energy Technology Laboratory
Katie Jo Sunday, Drexel University

Soft Magnetic Materials II
Thomas G. Woodcock, IFW Dresden
Orlando Rios, Oak Ridge National Laboratory

Sustainable Energy and Layered Double Hydroxides

High-Temperature Systems for Energy Conversion and Storage
Solid Oxide Fuel Cell: Recent Developments I
Paul Ohodnicki, National Energy Technology Laboratory
Kyle Brinkman, Clemson University

High Temperature Ceramic Materials: Response, Modelling and Performance
Amit Shyam, Oak Ridge National Laboratory
Kathy Lu, Virginia Tech

Solid Oxide Fuel Cell: Recent Developments II
Paul Ohodnicki, National Energy Technology Laboratory
Amit Pandey, Rolls Royce LG Fuel Cell Systems Inc.

Innovation in Energy Conversion and Storage I
Soumendra Basu, Boston University
Jung Choi, Pacific Northwest National Laboratory
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ENERGY TECHNOLOGIES AND CARBON DIOXIDE MANAGEMENT SYMPOSIUM 2015

Carbon Management

Session Chairs:
Animesh Jha
Cynthia K. Belt
A THERMODYNAMIC STUDY OF MIXED CARBON FEEDSTOCK GASIFICATION SLAGS

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Keywords: Phase diagram, Equilibrium, Gasification, Coal, Petroleum coke, Additive agents

Abstract

Integrated Gasification Combined Cycle used in power and chemical production is considered a clean technology, with the ability to capture almost all CO2, NOx, and SOx emissions. In entrained bed slagging gasifiers, molten slags formed from feedstock’s non-volatile impurities contribute to gasifier liner degradation and can cause gasifier clogging, affecting system efficiency and operation. Increased petcoke use as a key feedstock in addition to or as a replacement for coal has drastically modified slag chemistry, leading to unknown chemical/physical slag properties and behavior in the gasifier. In this work, thermodynamic phase equilibria in synthetic slags (Al2O3-CaO-FeO-SiO2-V2O3) were evaluated under simulated gasifier conditions to establish an understanding of the phase equilibrium in these slag systems. The effects of V2O3 content, slag chemistry, and additives on amorphous and crystalline phases were studied. In this study, increasing calcium oxide and iron oxide additive agents was found to lower the slag melting temperature and caused the karelianite (V2O3) crystal size to increase. Equilibrium phase diagrams showing the additive effect on the mixed coal-petcoke slag systems studied were constructed.

Introduction

Integrated Gasification Combined Cycle (IGCC) [1, 2] is a clean technology for chemical and power production, with almost all the harmful emissions effectively captured. During IGCC operation, synthesis gas (syngas) is produced, which consists primarily of hydrogen (H2) and carbon monoxide (CO). H2 and CO are used as fuel in turbines generating power or as a feedstock in chemical production. In entrained flow slagging gasifiers, non-volatile impurities from feedstock ashes form molten slag, which promotes refractory liner degradation and potential gasifier clogging problems. Sufficient slag fluidity, controlled by gasifier temperature, facilitates a downward slag flow toward the exit along the refractory lining of the gasification chamber. As a result, molten slag continuously interacts with the refractory materials. Typical operation temperatures for the entrained flow slagging gasifiers are in the range of 1325 - 1575 °C, with a 10^9 to 10^7 atm oxygen partial pressure [3]. Currently, petroleum coke (petcoke) feedstock is used as an economical additive or alternative to coal feedstock. The chemistry of the resulting slag is significantly different from coal gasifier slags due to the high vanadium...
content of petcoke ashes, which leads to uncertainty in gasifier performance. To optimize
gasifier design and operation, understanding of the thermodynamic nature of the vanadium-rich
slags is important. However, there is no commercially available thermodynamic database for
vanadium-containing slags. Chemical composition ranges of selected ash constituents found in
the U.S. and Canada are summarized in Table 1.

Table 1. Chemistries of industrial coal and petcoke ashes found in the U.S. and Canada

<table>
<thead>
<tr>
<th>Ash component</th>
<th>Coal ash</th>
<th>Petcoke ash</th>
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<tbody>
<tr>
<td></td>
<td>U.S.</td>
<td>Canada</td>
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<td>Reference</td>
<td>[4]</td>
<td>[7, 8]</td>
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<tr>
<td>Al_{2}O_{3}</td>
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<td>CaO</td>
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<td>Fe_{2}O_{3}</td>
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<td>NiO</td>
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<tr>
<td>P_{2}O_{5}</td>
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<tr>
<td>SiO_{2}</td>
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<td>SO_{3}</td>
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<td>TiO_{2}</td>
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<tr>
<td>V_{2}O_{5}</td>
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<tr>
<td>Total</td>
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<td>97.1</td>
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<tr>
<td>SiO_{2}/Al_{2}O_{3}</td>
<td>1.73</td>
<td>2.79</td>
</tr>
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</table>

U.S. coal ash chemical data represents 300 coal samples across the U.S.[4]. Chemistries of U.S.
petcoke ashes are reported from delayed coke, shot coke, fluid coke, and flexicoke [5] and [6].
Canadian coal ash compositions are representative of Canadian thermal coals: sub-bituminous
coals from Alberta, lignite coal from Saskatchewan and bituminous coals in use in Nova Scotia
[7, 8]. Canadian petcoke ash compositions [9, 10] are typical of delayed and fluid cokes from
Alberta oil sands operations and petcoke in use at an eastern Canadian power utility.

Phase equilibria for steelmaking slag systems containing vanadium have been reported in the
literature [11, 12] and for the Al_{2}O_{3}-CaO-V_{2}O_{5} system [13]. In previous work [3] an equilibrium
study of the Al_{2}O_{3}-CaO-FeO-SiO_{2}-V_{2}O_{5} system was first conducted at 1500 °C in 10^{-8} atm of