



VIRTUAL



SOLAR ENERGY SYSTEMS CONFERENCE

August 12 – 14, 2020

Organized by the Center for Energy Initiatives

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TIPS FOR A SUCCESSFUL MEETING



Say **hello** to everyone.
You might make someone's day.



Introduce yourself to people you don't know.
They may be your next good friends.



Stop and **smile**.
You will brighten the room considerably.



Be **understanding**.
Everybody makes mistakes.



Help those with less experience.
We were all novices at some point.



Respect others.
We all have something valuable to contribute.



Value staff and volunteers.
They are here for you.



Be **kind**.
You will never like everybody, but you can be cordial to all.



Enjoy the meeting!
You can have fun while sharing, learning and networking.

Abstracts appear as submitted by their authors. Neither the American Institute of Chemical Engineers (AIChE) and its entities, nor the employers affiliated with the authors or presenting speakers, are responsible for the content of the abstracts.

WELCOME ADDRESS

Welcome!

We would like to personally welcome you to the Virtual 2020 Solar Energy Systems Conference (Solar 2020) brought to you by the Center for Energy Initiatives (CEI), an American Institute of Chemical Engineers (AIChE) technological community, and hosted by Pathable.

The 2020 Solar Energy Systems Conference will focus on innovations to materials discovery, solar reactor design and modeling, systems-scale analyses, and commercialization activities on the broad topics pertinent to solar energy systems. For this year, we have three keynote talks, 12 invited speakers and panelists, and several selected oral presentations on the topics of: (a) high- and low-temperature solar fuel generators; (b) thermal energy storage; (c) solar energy for process heat and water treatment; and (d) process and systems modeling. In the second edition of this conference, we have also introduced panel discussions to facilitate active engagement between the broader audience, scientific and industrial experts, and government funding agencies.

The last several months have brought an extraordinary set of hardships. Much has changed about how all of us go about our daily routines and we are having to quickly adapt to constantly changing circumstances. We would like to express our appreciation for the way the engineering and the scientific community has come together in the face of these challenges. There is much to be impressed and inspired by the creativity, ingenuity, and care shown by people from all walks of life to keep the essence, authenticity, and spirit of progress alive and well. What happens next is crucial for our energy future, and some of us have the luxury and resources to think about the future and work to do our parts. Scientific collaboration and breakthroughs in the fields of renewable energy and sustainability are now more critical than ever before. The CEI will continue to meet, even if virtually, to bring encourage exchange of ideas and to bring motivated people together to ensure that energy research remains at the cutting edge.

A lot of work has gone into making this conference a success. We extend our sincere appreciation to the *AIChE organizing staff*, especially Lucy Alexander and Mahfuzul Islam, for doing the groundwork and taking care of all the administrative tasks required to run this conference smoothly. We thank the contributions of the members of the *Steering Committee* for their active participation in planning for and running the conference sessions and panels. We would also like to thank each and every one of the *distinguished speakers and panelists* for seamlessly adapting to the virtual format and being willing to share their expertise as part of our conference.

Finally, thanks to each of you for attending this conference and bringing your expertise and energy to this gathering. Throughout this conference, we ask you to stay engaged, be proactive, and help shape the future of the world. We hope your experience is a pleasant, educational, and an inspiring one.

Sincerely,

Conference Chair of Solar 2020

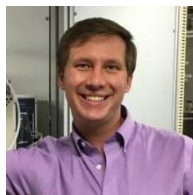


Rohini Bala Chandran
Assistant Professor
University of Michigan

and Conference Co-Chairs of Solar 2020



Nick AuYeung
Assistant Professor
Oregon State University



Christopher Muhich
Assistant Professor
Arizona State University

CONFERENCE ORGANIZERS

Conference Chair

[Rohini Bala Chandran - University of Michigan](#)

Conference Co-Chairs

[Nick Auyeung - Oregon State University](#)

[Christopher Muhich - Arizona State University](#)

Steering Committee

[Andrej Lenert - University of Michigan](#)

[Meng Lin - Southern University of Science and Technology in China](#)

[Erik Koepf - DuPont's Silicon Valley Technology Center](#)

[Clifford Ho - Sandia National Laboratories](#)

[Matthew Bauer - U.S. Department of Energy \(DOE\)](#)

[Chiranjeev Kalra - IdeaLab Studio](#)

Organized by



TECHNICAL PROGRAM

ALL TIMES ARE IN EASTERN STANDARD TIME (EST)

Wednesday, August 12	
1:00 - 1:05 PM	Opening and Welcome
1:05 - 1:40 PM	Keynote 1 & Q&A
	Moderator: Meng Lin, Southern University of Science and Technology in China and Rohini Bala Chandran, University of Michigan Chengxiang Xiang, California Institute of Technology . <i>Keynote Talk: Fuels from Sunlight: Multi-Physics Modeling, Materials Discovery and Prototype Development</i>
1:40 - 1:45 PM	Break
1:45 - 2:45 PM	Technical Session 1 - Thermal Energy Storage 1
	Session Chair: Andrej Lenert, University of Michigan .
1:45 - 2:00 PM	Craig Turchi, National Renewable Energy Laboratory . <i>Invited Talk: Liquid Pathway to SunShot: High-Temperature Liquids and Their Use in Next Generation Concentrating Solar Power Systems</i>
2:00 - 2:15 PM	Hadi Ghasemi, University of Houston. <i>Invited Talk: Full Spectrum Solar Thermal Energy Harvesting and Storage By a Molecular and Phase-Change Hybrid Material</i>
2:15 - 2:25 PM	Jesse R. Fosheim, Colorado School of Mines. <i>Narrow-Channel Fluidized Beds for Particle-sCO₂ Heat Exchangers in Next Generation CSP Plants</i>
2:25 - 2:35 PM	Nipun Goel, Boise State University. <i>High Temperature Erosion in Particle Based CSP Systems</i>
2:35 - 2:45 PM	Lin Zhao, Massachusetts Institute of Technology. <i>Ultra-Transparent Silica Aerogel for Solar Thermal Energy Systems</i>
2:45 - 3:00 PM	Q&A Session and Networking Break
3:00 - 4:00 PM	Panel Discussion 1 - Thermal Energy Storage
	Moderator: Nick AuYeung, Oregon State University .
	Matt Bauer, U.S. Department of Energy .
	Clifford Ho, Sandia National Laboratories .
	James Klausner, Michigan State University .
	Joerg Petrasch, Michigan State University .
	Mahesh B. Venkataraman, 1414 Degrees Ltd.
4:00 - 4:05 PM	Break
4:05 - 5:15 PM	Technical Session 2 - Solar Fuels 1
	Session Chair: Rohini Bala Chandran, University of Michigan
4:05 - 4:20 PM	Shane Ardo, University of California, Irvine . <i>Invited Talk: Design guidelines for photocatalyst reactors for solar fuels production based on numerical simulations and composite materials engineering</i>
4:20 - 4:35 PM	Todd G. Deutsch, NREL . <i>Invited Talk: Practical Challenges in Scaling III-V Semiconductor-Based Solar Hydrogen Systems</i>
4:35 - 4:45 PM	Meng Lin, Southern University of Science and Technology . <i>Towards 10% Solar-to-Hydrogen Efficiency of Ceria-Based Thermochemical Cycle Assisted with Electrochemical Oxygen Pump</i>

TECHNICAL PROGRAM

4:45 - 4:55 PM	Keisuke Obata, Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH. <i>Modeling and in-Situ Monitoring of Local pH Gradient during Near-Neutral Electrochemical Water Splitting</i>
4:55 - 5:05 PM	Sha Li, The Australian National University. <i>Numerical Modelling of Ceria Undergoing Reduction in a Particle–Gas Counter-Flow: Effects of Chemical Kinetics Under Isothermal Condition</i>
5:05 - 5:15 PM	Da Xu, Southern University of Science and Technology. <i>Exploring Gradient Functional Material for Enhanced Performance of Solar-Driven Thermochemical Fuel Production</i>
5:15 - 5:30 PM	Q&A Session and Networking Break
5:25 - 6:00 PM	Happy Hour and Open Mic
Thursday, August 13	
12:30 - 1:00 PM	Introduction to RAPID Manufacturing Institute
1:00 - 1:05 PM	Welcome and Last Day's Takeaways
1:05 - 1:40 PM	Keynote 2 & Q&A
	Moderator: Christopher Muhich, Arizona State University
	Martin Roeb, DLR (German Aerospace Center). <i>Keynote Talk: Processes for Solar Thermochemical Fuel and Commodity Production</i>
1:40 - 1:45 PM	Break
1:45 - 2:35 PM	Technical Session 3 - Thermal Energy Storage 2
	Session Chair: Clifford Ho, Sandia National Laboratories.
1:45 - 1:55 PM	James Yates, Job Industrial Services. <i>Design Path and Challenges of a Next-Generation, Refractory-Lined, Molten-Salt Storage Tank</i>
1:55 - 2:05 PM	Sean Lubner, Lawrence Berkeley National Lab. <i>Long Duration Thermal Energy Storage Using Thermo-Photovoltaics and Solid Storage Media</i>
2:05 - 2:15 PM	Bingjia Li, University of Michigan. <i>On the Influence of Spatial Correlations on Radiative Transport in Particulate Media</i>
2:15 - 2:25 PM	Jian Zeng, University of California, San Diego. <i>High-Temperature Measurement of Thermophysical Properties of Bulk Material and Coating Using Modulated Photothermal Radiometry</i>
2:25 - 2:35 PM	Mike Mayer, University of Michigan. <i>Thermal Radiative Property Measurements of Particulate Media</i>
2:35 - 2:50 PM	Q&A Session and Networking Break
2:50 - 3:50 PM	Panel Discussion 2 - Advances, Opportunities and Challenges in Solar and Electrochemical Fuel Technologies
	Moderators: Christopher Muhich, Arizona State University and Rohini Bala Chandran, University of Michigan
	Zeitan Mi, University of Michigan
	Alan Weimer, University of Colorado
	Andrea Ambrosini, Sandia National Lab
	Paul Kenis, University of Illinois
3:50 - 3:55 PM	Break
3:55 - 4:45 PM	Technical Session 4 - Solar Fuels & Solar Thermochemical Energy Storage

TECHNICAL PROGRAM

	Session Chair: Christopher Muhich, Arizona State University
3:55 - 4:10 PM	Ellen B. Stechel, Arizona State University . <i>Invited Talk: Materials Thermodynamic Limits in Solar-Thermochemical Fuel Production</i>
4:10 - 4:25 PM	Nick AuYeung, Oregon State University . <i>Invited Talk: Future Direction and Challenges for Solar Thermochemical Energy Storage</i>
4:25 - 4:35 PM	Jayni Hashimoto, Arizona State University. <i>The Thermodynamics of Magnesium Manganate Reduction for Application in Thermochemical Energy Storage Systems</i>
4:35 - 4:45 PM	Bo Wang, The Australian National University. <i>Thermal Reduction of Iron-Manganese Oxide Particles in a High-Temperature Packed-Bed Reactor for Solar Thermochemical Energy Storage</i>
4:45 – 5:00 PM	Q&A Session and Networking Break
5:00 - 6:00 PM	RAPID Manufacturing Institute Interactive Workshop
Friday, August 14	
1:00 - 1:05 PM	Welcome and Last Day's Takeaways
1:05 - 1:40 PM	Keynote 3 & Q&A
	Moderator: Nick AuYeung, Oregon State University Ahmed Ghoniem, Massachusetts Institute of Technology . <i>Keynote Talk: Materials, Reactors and Systems for Efficient and Scalable Production of Solar Fuels Using Thermochemical Cycles</i>
1:40 - 1:45 PM	Break
1:45 - 2:45 PM	Technical Session 5 - Process, Systems and Materials Modeling
	Session Chair: Meng Lin, Southern University of Science and Technology in China
1:45 - 1:55 PM	Lifeng Li, The Australian National University. <i>Optical Analysis of a Novel Solar Thermochemical System with a Rotating Tower Reflector and a Receiver–Reactor Array</i>
1:55 - 2:05 PM	Jieyang Li, Southern University of Science and Technology. <i>Unified Design Guidelines for High Flux Solar Simulator with Controllable Flux Vector</i>
2:05 - 2:15 PM	Steven Wilson, Arizona State University. <i>Sorption Pumping of O₂ Pumping Using Alpo-5 Zeolites: A Density Functional Theory Study</i>
2:15 - 2:25 PM	Swapana S. Jerpoth, Rowan University. <i>Optimal Selection of Ions for Perovskite Solar Cell Synthesis through a Computational Approach</i>
2:25 - 2:35 PM	Konstantinos Kakosimos, Texas A&M University at Qatar. <i>Semi-Automatic Method to Optimize Multi-Lamp High Flux Solar Simulators Utilizing Machine Learning Algorithms</i>
2:35 - 2:45 PM	Zijie Chen, University of Michigan. <i>Using Monte Carlo Ray Tracing and Data-Driven Techniques for Radiative Transport in Particulate Media</i>
2:45 - 3:00 PM	Q&A Session and Networking Break
3:00 - 4:00 PM	Panel Discussion 3: Funding Opportunities
	Moderator: Andrej Lenert, University of Michigan
	Bhima Sastri, National Energy Technology Laboratory
	Matt Bauer, U.S. Department of Energy Ying Sun, National Science Foundation

TECHNICAL PROGRAM

	Michael Haney, ARPA-E, U. S. Department of Energy
4:00 - 4:05 PM	Break
	Technical Session 6 - Solar Process Heat/ Water Treatment
4:05 - 5:35 PM	Session Chair: Chiranjeev Kalra, IdeaLab Studio and Solomon Adera, University of Michigan
4:05 - 4:20 PM	Akanksha Menon, Lawrence Berkeley National Lab. <i>Invited Talk: Efficient Utilization of Solar Energy for Wastewater Treatment Via Radiative Heating</i>
4:20 - 4:35 PM	Brandon Hathaway, Sunvapor. <i>Invited Talk: Techno-economic Analysis of SCEPTRE – Solar Cascading Evaporation Process to Recover Effluent</i>
4:35 - 4:45 PM	Trevor Demayo, Chevron. <i>Lost Hills Solar - Powering an Oil and Gas Field with Renewable Energy</i>
4:45 - 4:55 PM	Luisa Barrera, University of Michigan. <i>Effects of Competing Reactions and Effluent Stream Composition on the Energy Efficiency of a Photoelectrochemical Wastewater Nitrate Treatment Device</i>
4:55 - 5:05 PM	Alejandro Espejo Sanchez, Boise State University. <i>Modeling of a Hybrid Membrane Distillation/ Photovoltaic Cell</i>
5:05 - 5:15 PM	Dario Pardillos Pobo, University Carlos III of Madrid. <i>Modelling a Conveyor-Belt Solar Receiver to Dry and Heat Aggregates in Hot Mix Asphalt Industry</i>
5:15 - 5:25 PM	Jingyi Zhang, Northwestern University. <i>Technical Potential and Environmental Impact Assessment of PV Electric Powered Industrial Process Heating</i>
5:25 - 5:35 PM	Carrie Schoeneberger, Northwestern University. <i>Solar Industrial Process Heating: A Technical Potential Analysis for U.S. Manufacturing</i>
5:35 - 5:50 PM	Q&A Session and Networking Break
5:50 - 6:00 PM	Closing Remarks

Latest complete conference information available at www.aiche.org/solar

KEYNOTE SPEAKER BIOGRAPHIES

Keynote Speaker Biography



Ahmed Ghoniem

Massachusetts Institute of Technology

Ahmed Ghoniem is the Ronald C. Crane Professor of Mechanical Engineering, Director of the Center for Energy and Propulsion Research and the Reacting Gas Dynamics Laboratory at MIT. He received his B.Sc. and M.Sc. degree from Cairo University, and Ph.D. at the University of California, Berkeley. His research covers computational engineering with application to turbulence and combustion, multiphase flow and multiscale phenomena, clean energy technologies with focus on CO₂ capture, renewable energy and alternative fuels. His research has made fundamental contributions to multiscale simulations, thermochemistry, combustion dynamics, energy systems and materials chemistry. He supervised more than 100 M.Sc., Ph.D. and post-doctoral students, many are leaders in academia, industry and governments; published more than 500 refereed articles in leading journals and conferences; lectured extensively around the World; and consulted for the aerospace, automotive and energy industry. He is fellow of the American Society of Mechanical Engineer (ASME), the American Institute of Physics (APS), the Combustion Institute (CI), and associate fellow of the American Institute of Aeronautics and Astronautics (AIAA). He received several prestigious awards including the ASME James Harry Potter Award in Thermodynamics, the AIAA Propellant and Combustion Award, the KAUST Investigator Award and the Committed to “Committed to Caring Professor” at MIT. He is currently the MIT PI of the Center of Excellence for Energy, a \$30M effort to improve energy research, education and entrepreneurship in Egypt.



Martin Roeb

German Aerospace Center (DLR)

Dr. Martin Roeb holds a diploma in chemistry from the University of Cologne and a doctoral degree in physical chemistry from the same university. Since 1999 he has been working as a scientist, project manager and group leader in DLR’s Solar Research Division in the field of solar high temperature applications. He took over the lead of the team “high temperature solar chemical engineering” in 2010. He has been work package leader and coordinator of several domestic and EU projects on solar high temperature processes and in particular on solar fuels. His research interests address processes and materials related to solar thermochemical water and CO₂ splitting, solar upgrading of hydrocarbons, high temperature electrolysis and solar recycling and production processes of chemical commodities. He has been involved in international cooperation in the context of EERA, IEA, the IPHE and SOLARPACES. He used to be the DLR representative in the project HYDROSOL, which has been awarded by the Eco Tech Award Expo 2005, the Technical Achievement Award of the International Partnership for the Hydrogen Economy 2006 and the Descartes Prize 2006 for Scientific Collaborative Research.

KEYNOTE SPEAKER BIOGRAPHIES



Chengxiang Xiang
California Institute of Technology

Dr. Chengxiang (“CX”) Xiang is a Principal Investigator and Staff Scientist in Joint Center for Artificial Photosynthesis (JCAP) at California Institute of Technology. Dr. Xiang received his Ph. D in Chemical and Material Physics in University of California, Irvine in 2009 with Prof. Reginald M. Penner. Dr. Xiang was then a Postdoctoral Scholar for Prof. Nate Lewis at the California Institute of Technology from 2009 to 2011. Dr. Xiang research interests include design and fabrication of high efficiency solar-fuel prototypes, high throughput materials discovery, opto-electronic-catalytic modeling of advanced micro/nanostructured photoelectrochemical systems and multi-ion transport modeling in solution and polymer electrolytes. (<http://sunlight.caltech.edu/cx/>)

INVITED SPEAKER BIOGRAPHIES

Invited Speaker Biographies



Matthew Bauer

U.S. Department of Energy (DOE)

Matthew develops and manages R&D initiatives for the Solar Energy Technologies Office's (SETO) Concentrating Solar Thermal Power (CSP) program. In this capacity, novel technologies are identified and de-risked to enable widespread deployment of CSP and related thermal systems. Matthew has been with SETO since 2015 developing initiatives including grid firming thermal energy storage, Gen 3 CSP, particle based solar thermal technologies, sCO₂ power cycle development, solar thermal desalination, and novel metrology for CSP. Matthews research background is in the field of microscale heat transfer. This includes the development of heat transfer metrology techniques for multiphase nano- to microscale material systems. He holds a Ph.D. in Mechanical Engineering from the University of Virginia, and a B.S. in Mechanical Engineering from Christian Brothers University.



Shane Ardo

University of California Irvine, Irvine, California, USA

Shane obtained a B.S. Degree in Mathematics and a minor in Computer Programming from Towson University, an M.S. Degree in Nutrition from the University of Maryland, College Park, and a Ph.D. Degree (2010) in Photo-Physical Inorganic Chemistry from the Johns Hopkins University under the guidance of Prof. Jerry Meyer. He then worked as a DOE–EERE Postdoctoral Research Awardee at the California Institute of Technology under the guidance of Prof. Nate Lewis until 2013. Since that time, Shane has been an Assistant Professor (2013 – 2019) and now a tenured Associate Professor at the University of California Irvine in the Department of Chemistry, and holds courtesy joint appointments in the Departments of Chemical & Biomolecular Engineering and Materials Science & Engineering. The Ardo Group has expertise in experimental and theoretical photochemistry and electrochemistry, and they use knowledge from those fields to design and control spatiotemporal mechanisms and dynamics of non-equilibrium processes relevant to desalination, atmospheric water harvesting, solar fuels, and electrolyzers. In 2016, Shane was named one of five inaugural Moore Inventor Fellows. He is also a recipient of a DOE Early Career Research Award and two Beall Innovation Awards, and was named a Sloan Research Fellow, a Cottrell Scholar, a Kavli Fellow, and a Scialog Fellow. The Ardo Group is also supported by funding from the DOE Office of Energy Efficiency and Renewable Energy, Nissan Chemical Corporation, and Research Corporation for Science Advancement, and they are members of the DOE Energy–Water Desalination Hub.

INVITED SPEAKER BIOGRAPHIES



Todd Deutsch
National Renewable Energy Laboratory

Dr. Deutsch performed his graduate studies on III-V semiconductor water-splitting systems under the joint guidance of Dr. John Turner (NREL) and Prof. Carl Koval in the Chemistry department at the University of Colorado-Boulder. He officially joined NREL as a postdoctoral scholar in Dr. Turner's group in 2006 and became a staff scientist two years later. Since 2014, he has led NREL's applied water splitting program that aims to identify and characterize appropriate materials for economically generating hydrogen fuel from water using sunlight as the only energy input. His work has focused on inverted metamorphic multijunction III-V semiconductors and corrosion remediation strategies for high-efficiency water-splitting photoelectrodes. In the last couple years he been funded to develop advanced bipolar membranes for reversible fuel cells and CO₂ electrolyzers. The CO₂ electrolyzer project is a multi-lab program that aims to invent CO₂ electrolyzers that can electrocatalytically reduce CO₂ to useful chemicals and fuels at industrially-relevant rates. Dr. Deutsch has been honored as an Outstanding Mentor by the United States Department of Energy, Office of Science nine times in recognition of his work as an advisor to over thirty students in the Science Undergraduate Laboratory Internship program at NREL. He received a B.S. in Chemistry, cum laude, from Humboldt State University and a Ph.D. in Analytical Chemistry from the University of Colorado-Boulder.



Clifford Ho
Sandia National Laboratories

Dr. Cliff Ho is a Fellow of the American Society of Mechanical Engineers and a Senior Scientist at Sandia National Laboratories, where he has worked since 1993 on problems involving solar energy, energy storage, water safety and sustainability, heat- and mass-transfer processes in porous media, and microchemical sensor systems for environmental monitoring. He holds 15 patents, has published over 300 scientific papers, and is an Associate Editor of Elsevier's Solar Energy Journal. Dr. Ho is the recipient of two R&D 100 Awards, an outstanding professor award, the national Asian American Engineer of the Year award, and the first-place award in Discover Magazine's "Future of Energy in Two-Minutes-or-Less Video Contest." He received his B.S. in Mechanical Engineering from the University of Wisconsin-Madison in 1989, and his Master's and Ph.D. in Mechanical Engineering from the University of California at Berkeley in 1990 and 1993.



James Klausner
Michigan State University

James Klausner's research interests focus on thermal, chemical, and fluid transport in a variety of applications including, energy, processing, thermal management, desalination, powder flow, cryogenics, and bioengineering. He has done extensive fundamental work on the dynamics of phase change phenomena, including nucleation and bubble dynamics. He is very interested in sustainable engineering processes and is currently working on using sunlight, water, recycled CO₂, and biomass as

INVITED SPEAKER BIOGRAPHIES

possible inputs to thermochemical reactors for synthetic fuel production, such as hydrogen and higher order hydrocarbons as the output. Highly concentrated solar radiation is used to drive high temperature thermo-chemical conversion processes. He is also working on using low grade waste heat and un-concentrated solar energy for low temperature desalination. He has developed a number of phase-change thermal management processes that operate at unprecedented heat fluxes. He has a strong interest in light metals processing and energy efficient advanced manufacturing. He has nine patents and copyrights that resulted from his research work.



Akanksha Krishnakumar Menon
Lawrence Berkeley National Laboratory

Akanksha Menon is an ITRI-Rosenfeld Postdoctoral Fellow in the Prasher group. Her research interests are in the water-energy nexus, specifically on energy-efficient water desalination techniques. At Berkeley Lab, Akanksha is focused on treating high salinity waters by using solar energy and novel membrane processes, with the goal of achieving zero liquid discharge and closing the water loop. Akanksha obtained her Ph.D. in Mechanical Engineering from Georgia Tech in 2018, where she focused on developing polymer thermoelectric materials and devices for energy harvesting. Akanksha is a recipient of the 2017 MRS Graduate Student Award and has served as the Co-President of the Energy Club @ Georgia Tech.



Joerg Petrasch
Michigan State University

Joerg Petrasch received his M.S. and PhD from the Department of Mechanical and Process Engineering at ETH Zurich, Switzerland. He completed his PhD research on the tomography-based modeling of reactive flows in porous structures applied to solar chemical fuel production in 2007. He has worked as a numerical analyst and consulting engineer in the chemical, construction, and energy industries. In 2009 he joined the faculty of the University of Florida as an Assistant Professor. There, he helped to build a successful solar thermochemistry program. Between 2012 and 2017 he was the Illwerke-VKW Founding Professor for Energy Efficiency and Director of the Energy Research Center at the Vorarlberg University of Applied Sciences (FHV), Austria. In this role, he was responsible for initializing, developing, and building the energy program. After a stint as an entrepreneur running his own process engineering company from 2017 to 2018, Dr. Petrasch is currently an Associate Professor at MSU. His research interests are: chemical storage of renewable energy, tomography-based numerical and experimental methods for energy applications, micro-structured functional materials for energy applications as well as demand side management, control, and short-term buffering of sustainably generated energy.



Bhima Sastri
National Energy Technology Laboratory

INVITED SPEAKER BIOGRAPHIES

Dr. Bhima Sastri is the Division Director of Crosscutting R&D and Systems Integration, Office of Fossil Energy, U.S. Department of Energy. He overlooks R&D funding for several technology areas including the Coal FIRST (Flexible, Innovative, Resilient, Small, and Transformative) Initiative, Energy Storage, Supercritical CO₂ program, Institute for the Design of Advanced Energy Systems (IDEAS), and several crosscutting programs such as the University Turbine Research (UTR) program and the Historically Black Colleges and Universities (HBCU) programs. He has over 20 years of experience in research and development of chemical and energy technologies. Before joining the Fossil Energy Office, he was with the Advanced Manufacturing Office at DOE where he managed the Advanced Chemical Separations, Desalination, and Bio-Manufacturing technology portfolios. He is currently on the executive board of the RAPID which is the Modular Chemical Process Intensification Institute for Clean Energy Manufacturing.

Dr. Sastri completed his Ph.D. in Chemical Engineering from Rensselaer Polytechnic Institute, Troy, NY and a B.S. in Chemical Engineering from IIT Madras. For over 15 years prior to joining DOE, he worked in private industry as a General Manager of R&D and as a Senior Research Engineer and has held visiting faculty positions at different universities where he taught undergraduate chemical engineering courses.



Ellen Stechel
Arizona State University

Ellen B Stechel is Co-Director, ASU LightWorks[®]; Professor of Practice, School of Molecular Sciences; and Senior Sustainability Scientist, Julie Ann Wrigley Global Institute of Sustainability at Arizona State University (ASU.) Her career has afforded her opportunities to build and/or coordinate research programs at a national laboratory, industry, a U.S. government agency, and now in higher education at ASU; in both basic and applied research; policy and commercialization of emerging technologies; and in multi-disciplinary R&D strategy and management. She has held and holds numerous positions of an advisory or editorial capacity nationally and internationally and has published >100 peer reviewed articles. Her current research focuses on materials and systems design for concentrating solar technologies for producing sustainable liquid hydrocarbons from carbon dioxide, hydrogen from advanced water splitting, clean water, renewable ammonia, and for thermochemical energy storage.



Ying Sun
National Science Foundation

Dr. Ying Sun is the Program Director of the Thermal Transport Processes Program in the Directorate for Engineering at the National Science Foundation. The program supports fundamental and transformative research in thermodynamics, and heat and mass transfer. Dr. Sun is also a Professor in the Department of Mechanical Engineering and Mechanics at Drexel University. Her research interests include multiphase flows and heat/mass transfer, complex fluids, and multiscale modeling with applications in energy systems and advanced manufacturing. She was a recipient of the NSF CAREER Award, AFOSR Summer Faculty Fellowship, French CNRS Visiting Professorship, and Drexel College of Engineering Research Achievement Award. She was an ELATE Leadership Fellow and a visiting professor at Princeton University, Ecole Polytechnique, and Tsinghua University. Dr. Sun serves as an Associate Editor for ASME Journal of Electrochemical Energy Conversion and Storage.

INVITED SPEAKER BIOGRAPHIES



Craig Turchi

National Renewable Energy Laboratory

Dr. Turchi has been investigating solar thermal and geothermal technologies at NREL for the past twelve years, where he currently leads NREL's Thermal Energy Science & Technologies Group and assists with the development and assessment of heat-transfer fluids, thermal-storage concepts, and advanced power systems. He was responsible for development of several of the Concentrating Solar Power (CSP) technology metrics associated with the DOE's SunShot Initiative to drive down the cost of solar energy and has championed the development of supercritical-CO₂ power systems for CSP applications.

KEYNOTE 1

Keynote Talk: Fuels from Sunlight: Multi-Physics Modeling, Materials Discovery and Prototype Development.

Chengxiang Xiang

Joint Center for Artificial Photosynthesis, California Institute of Technology, Pasadena, CA

As the level of penetration for the renewable energy sources continues to rise, large-scale, long-term energy storage technologies that could time-shift the usage of the energy daily or seasonally starts to play a significant role in the overall development and deployment of renewable energies. One approach to compensate for the intermittency of sunlight on the surface of the earth is to store solar energy in the form of chemical bonds, i.e., in an artificial photosynthetic process.

Development of efficient artificial photosynthesis devices requires materials discoveries as well as synthetic assembly these materials, including light absorbers, electrocatalysts, membrane separators and electrolytes. In this talk, I will showcase recent research and developments in Joint Center for Artificial Photosynthesis (JCAP). I will first present a robust multi-physics, multi-dimensional device model that was used to guide the materials discovery, to define operational conditions and constraints and to optimize and explore novel device architectures for solar-driven water-splitting devices as well as solar-driven CO₂ reduction devices. Then, I will present high throughput synthesis and screening tools that were developed to search for new light absorbers and electrocatalysts materials for solar-fuel applications. Through the modeling guided prototype development and through the materials discovery efforts, a range of stable and intrinsically safe solar-driven hydrogen generating devices with >10% conversion efficiency have been assembled and characterized. Recently, we have also demonstrated a direct coupled, proof-of-concept electrochemical system that used a bipolar membrane electro dialysis (BPMED) cell and a vapor-fed CO₂R cell for electrochemical capture and conversion of CO₂ from oceanwater. The oceanic CO₂ capture and conversion system exhibited a record low electrochemical energy consumption of 155.4 kJ mol⁻¹ or 0.98 kWh kg⁻¹ of CO₂ and a Faradaic efficiency (FE) of up to 95% for electrochemical CO₂ reduction to CO.

TECHNICAL SESSION 1: THERMAL ENERGY STORAGE 1

Invited Talk: Liquid Pathway to SunShot: High-Temperature Liquids and Their Use in Next Generation Concentrating Solar Power Systems.

Turchi Craig

National Renewable Energy Laboratory, Golden, CO

NREL is leading a multi-national team to design and test the next generation of concentrating solar power (CSP) technology using high-temperature heat transfer and energy storage liquids. The cost-shared project will demonstrate the ability to deploy a molten-chloride salt for energy storage coupled with a liquid-metal sodium solar receiver for solar collection efficiency. This presentation will review the design of the 1-MWt pilot-scale system that will be proposed to the U.S. Department of Energy for construction and operation in project Phase 3. The system uses a ternary MgCl₂/KCl/NaCl energy-

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storage salt held in refractory-lined tanks. Sodium is used in the solar receiver and exchanges heat with the storage salt through a sodium-to-salt heat exchanger. The pilot unit will transfer thermal energy to supercritical carbon dioxide (sCO₂) to demonstrate a salt-to-sCO₂ heat exchanger operating at 700°C and mimic integration of a sCO₂ Brayton power cycle. The primary goal of the project is to design, develop, test, and validate at megawatt scale, a liquid-phase system consisting of the solar receiver, thermal energy storage (TES) unit, heat exchangers, and associated pumps, piping, valves, sensors, and controls.

Invited Talk: Full Spectrum Solar Thermal Energy Harvesting and Storage By a Molecular and Phase-Change Hybrid Material.

Varun Kashyap¹, Siwakorn Sakunkaewkasem¹, Randall Lee², and Hadi Ghasemi¹
(1)ME, University of Houston, Houston, TX, (2)Chemistry, University of Houston, Houston, TX

Efficient solar thermal energy harvesting and storage are critical steps toward utilizing the abundant solar irradiation that reaches the surface of the earth. Current solar thermal approaches rely on costly high optical concentration systems, leading to high heat losses by hot bulk materials and surfaces. At the same time, the energy stored in the form of thermal energy has inherently large temporal losses. Here, we combine the physics of molecular energy and latent heat storage to introduce an integrated, simultaneous harvesting and storage hybrid paradigm for potential 24/7 energy delivery. The hybrid paradigm utilizes heat localization during the day to provide a harvesting efficiency of 73% at small scale and ~90% at large scale. Remarkably, at night, the stored energy by the hybrid system is recovered with an efficiency of 80% and at a higher temperature than that of the day, in contrast to all of the state-of-the-art systems.

Narrow-Channel Fluidized Beds for Particle-sCO₂ Heat Exchangers in Next Generation CSP Plants.

Jesse R. Fosheim, Xavier Hernandez, Jeremy Abraham, and Gregory S. Jackson
Department of Mechanical Engineering, Colorado School of Mines, Golden, CO

Engineered alumina-silica particles provide a cost-effective solution for thermal energy storage (TES) and transport in next-generation concentrating solar power (CSP) plants that implement supercritical CO₂ (sCO₂) power cycles with temperatures above 700°C. Current particle-sCO₂ heat exchangers based on moving packed beds have high particle-wall thermal resistance ca. 4-5 m² K kW⁻¹, which result in large and costly primary heat exchangers. In contrast, bubbling fluidized beds have demonstrated the potential for much lower particle-wall thermal resistances < 1.0 m² K kW⁻¹ at conditions relevant for primary heat exchangers. Heat transfer measurements in a laboratory-scale narrow-channel fluidized bed test facility with CARBO Accucast ID50 ($d_p \approx 260 \mu\text{m}$) for operation up to 400°C and gas velocities to 0.55 m s⁻¹. A new particle-wall heat transfer correlation is developed that matches data over the full operating range within ±10%. Predicted particle-wall heat transfer coefficient exceeds 1000 W m⁻² K⁻¹ above 600°C. A quasi 1-D particle-sCO₂ heat exchanger model was developed in MATLAB to solve two-phase conservation equations in a narrow-channel fluidized bed with downward particle flow and to solve single-phase equations for countercurrent microchannel sCO₂ flows. The model, which incorporates experimentally fitted particle-wall heat transfer coefficients, was run to explore tradeoffs for a demonstration 40-kW_{th} heat exchanger design. With particle and sCO₂ inlets at 620°C and 450°C respectively, overall particle-sCO₂ heat transfer coefficients above 600 W m⁻² K⁻¹ were achievable at heat

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exchanger effectiveness > 80%. These results show that narrow-channel fluidized beds can enable small, cost-effective heat exchangers for future CSP plants.

High Temperature Erosion in Particle Based CSP Systems.

Nipun Goel¹, Tessa Mei-lin Fong¹, Evan Gietzen², Michael Keller², Siamack Shirazi³, and Todd Otanicar¹
(1)Mechanical and Biomedical Engineering, Boise State University, Boise, ID, (2)Mechanical Engineering, The University of Tulsa, Tulsa, OK, (3)Erosion/Corrosion Research Center, University of Tulsa, Tulsa, OK

Particle based concentrated solar power plants are increasingly being considered as an alternative to molten salts. Although these particle based systems provide the inherent safety and enhanced lifetime from reduced corrosion compared to molten salt systems, they bring in complexities associated with surface erosion from falling particle impact and sliding motion along the surfaces. Past research on particle related erosion has been limited to high velocity applications and doesn't necessarily coincide with the operating conditions in CSP systems.

In our work, we evaluate characterize the rate of erosion for particles and containment materials at 800°C. Three different types of erosion resulting from a) impact of solid particles on receiver, particle storage, and heat exchanger walls; b) abrasion erosion from particle sliding motion along walls; and c) attrition erosion as the particles breakdown from particle-to-particle contact and particle-to-wall interactions are evaluated and compared across a varied spectrum of particle and containment material spectrum.

From the results, It is noted that temperature plays a key role in the rate of erosion experienced by any material. With the increase in temperature, materials become more ductile and are more readily sheared away from particle impinging or sliding motion. Furthermore, the particles themselves have higher susceptibility to breakdown which also lowers particle thermal absorptance and thus efficiency as heat transfer fluid.

Ultra-Transparent Silica Aerogel for Solar Thermal Energy Systems.

Lin Zhao, Bikram Bhatia, Lenan Zhang, Elise Strobach, Sungwoo Yang, Thomas Cooper, Lee Weinstein, Gang Chen, and Evelyn Wang
Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA

Solar thermal energy systems provide a promising pathway to promote renewable energy as a source of electricity, heat, clean water, and chemical fuel. Thermal management, *i.e.*, minimizing heat loss in the solar-to-thermal conversion process, is a key field of research to enable next-generation efficient solar thermal technology. State-of-the-art systems utilize spectrally selective absorber, evacuated enclosure, and optical concentration to mitigate conductive, convective, and radiative heat loss. However, these components are expensive and require well-built infrastructures. In this work, we present an optimized ultra-transparent silica aerogel that can transmit >95% of the solar radiation while maintaining its thermally insulating properties. The microstructure of the silica aerogel is tailored to minimize light scattering in the solar spectrum and suppress heat transfer via conduction, convection, and radiation. With the developed aerogel, we demonstrated different prototype solar thermal systems with applications ranging from solar desalination, steam sterilization, industrial process heat, and power

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generation. For example, in an unconcentrated solar thermal collector, the developed aerogel enables stagnation temperature $>200^{\circ}\text{C}$ and provides extra driving force in a multistage solar still to boost water productivity. With a non-tracking compound parabolic concentrator (CPC), an aerogel collector can generate saturated steam at 125°C for medical sterilization even under hazy and cloudy skies. Finally, the aerogel can be integrated into a solar thermal receiver with linear Fresnel reflectors to enable efficient operations. In summary, the developed aerogel holds great potential to further promote solar thermal technology for a variety of applications.

PANEL DISCUSSION 1: THERMAL ENERGY STORAGE

Gen 3 Particle Pilot Plant (G3P3): Integrated High-Temperature Particle System for Concentrating Solar Power.

Clifford Ho

Sandia National Laboratories, Albuquerque, NM

This presentation will provide an overview of research efforts at Sandia National Laboratories to build a next-generation concentrating solar power (CSP) pilot plant using solid particles instead of a fluid as the heat-transfer and storage medium. The use of solid particles enables significant advantages over conventional molten nitrate salt CSP plants and other high-temperature systems employing gas as the heat-transfer fluid, including direct heating of the particles to reduce receiver infrastructure and start-up times, direct storage of the particles, no freezing, no need for hermetic seals, and the ability to achieve temperatures in excess of 1000°C . Challenges that are being researched include reduction of heat and particle losses from the open-aperture receiver; designs to increase particle-side heat-transfer coefficients in a high-temperature, high-pressure, moving-packed-bed particle-to-working-fluid heat exchanger; and designs for high-temperature particle storage and conveyance.

High Temperature Thermal Energy Storage Systems: Large Scale, Geography Independent and Cost Effective.

Mahesh B. Venkataraman, Nathan Levinson, Pan Vrettos, and Jordan Parham

1414 Degrees Ltd., Adelaide, SA, Australia

With the increase in the deployment of variable renewable energy generators, such as wind and solar PV, issues arise from the mismatch between the generation and demand profiles. Large-scale and cost-effective electricity storage is thus needed, in combination with demand-side management. Several commercial solutions exist for grid-scale electricity storage, e.g. batteries, pumped-hydro and compressed-air energy storage. However, each of these are limited by one or the other constraints such as scalability, geographical compatibility or cost. Thermal energy storage systems (TESS) could be a cost-effective and robust alternative to these commercial solutions.

A constant criticism of TESS has been its low round-trip efficiency. However, given that 8-10% of the world's total energy usage is in the form of high temperature heat ($>800^{\circ}\text{C}$), using TESS for electrical storage could be advantageous in reducing the carbon footprint of industrial processes such as cement making, iron-and-steel, hydrogen etc. 1414 Degrees' TESS technology uses Si-based alloys as phase-change materials, enabling clean, scalable and robust energy storage between $1000\text{--}1400^{\circ}\text{C}$. Our novel

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encapsulation technology eliminates the need for operation under vacuum or inert gas at high temperature and delivers a system which can operate under atmospheric air (or combustion environment in case of biogas as heating source). In this study, we will present the status of the thermal energy storage technologies, the versatility of TESS, cost-competitiveness with other storage options, challenges in downstream integration and key focus areas for future research.

TECHNICAL SESSION 2: SOLAR FUELS

Invited Talk: Design guidelines for photocatalyst reactors for solar fuels production based on numerical simulations and composite materials engineering.

Shane Ardo

Chemistry, University of California Irvine, Irvine, CA

Solar hydrogen production could be a techno-economically viable alternative to steam methane reforming through development of new reactor designs and reaction schemes. Motivated by this fact, my group recently proposed a dual-bed batch reactor for solar hydrogen production that contains stacked photocatalyst beds, which enable increases in efficiency due to serial light absorption and short distances for redox shuttle mass transport. An unexpected discovery based on this design is that an ensemble of optically thin materials is more beneficial to theoretical solar-to-hydrogen conversion efficiencies than a standard single-light-absorber geometry. Through parallel experimental work we have shown that state-of-the-art doped and codoped SrTiO₃ H₂-evolving photocatalyst particles exhibit variability in homogeneity of dopant distributions, which correlates to overall performance. We have also observed that carefully engineered nanoscale coatings on planar electrodes enable selective H₂ evolution and desired redox shuttle reactivity over undesired reactions. Collectively these results provide new design guidelines and additional research pathways for the development of effective composite materials to serve as active components in techno-economically viable solar fuels devices.

Invited Talk: Practical Challenges in Scaling III-V Semiconductor-Based Solar Hydrogen Systems.

Todd G. Deutsch, James L. Young, Walter E. Klein, and Myles A. Steiner
NREL, Golden, CO

While III-V semiconductors have achieved the highest photo-electrochemical solar-to-hydrogen conversion efficiencies, they are remarkably unstable during operation in a harsh electrolyte. The first part of this talk will focus on the degradation mechanism of inverted metamorphic multijunction (IMM) III-V cells and surface modification strategies aimed at protecting them from photocorrosion. We applied noble metal catalysts, oxide coatings by atomic layer deposition, and MoS₂ in an effort to protect the GaInP₂ surface that was in contact with acidic electrolyte. We also grew epitaxial capping layers from III-V alloys that should be more intrinsically stable than GaInP₂. The ability of the various modifications to protect the IMM's surface was evaluated by operating at each electrode at short circuit for extended periods of time.

The second part of this talk will identify the challenges encountered while scaling the IMM III-V absorber areas of from ~0.15 cm² up to 16 cm² and incorporating them in a photoreactor capable of generating three standard liters of hydrogen in eight hours under natural sunlight. To successfully scale photo-

electrochemical water-splitting technologies from bench to demonstration size requires addressing predictable and unpredictable complications. Despite using Comsol multiphysics to model our photoreactor and identify suitable specifications for a prototype, several practical issues were uncovered during testing that led to multiple iterations of photoreactor design between the initial and final generations. We faced many challenges to meeting our performance targets. Ultimately, the demonstration-scale system was able to generate nearly twice the target volume of hydrogen in an 8-hour outdoor trial.

Towards 10% Solar-to-Hydrogen Efficiency of Ceria-Based Thermochemical Cycle Assisted with Electrochemical Oxygen Pump.

Wandong Bai and Meng Lin

Department of Mechanical and Energy Engineering, Southern University of Science and Technology, Shenzhen, China

Solar-driven ceria-based thermochemical cycle is a promising route for renewable fuels production. Limited by large penalty of sweep gas, the solar-to-fuel (STF) efficiency from published literatures are < 7.5 %. In this study, we propose an efficient oxygen reduction technique based on a high-temperature electrochemical oxygen pump (EOP) to assist thermochemical reactor for hydrogen production. The EOP acts as a high-efficient oxygen removing device getting rid of the sweep gas and keeping at relative high pump efficiency.

We develop a transient 2D axial-symmetrical cell level model framework, which can well capture the coupled physics, including heat transfer across the whole reactor, fluid flow and species transport in porous ceria and electrodes domains, thermochemical reactions within the ceria domain, and electrochemical reactions at both electrodes of the oxygen pump. The developed numerical model offers a detail understanding of the reactor's transient behaviors under various design parameters and operation conditions. The impact of solar concentration, ceria thickness, operation voltage, and reaction kinetics are discussed in this study offering design guidelines for optimal reactor design and operation conditions.

The results show that the integrated solar reactor with the EOP can achieve higher oxygen release rate over reduction process leading increased STF efficiency compared to the case with sweep gas. With optimized design and operation parameters, an STF efficiency close to 10% can be achieved. This novel integrated electro-thermochemical reactor for showed potential for large scale engineering of high temperature thermochemical fuel production technologies.

Modeling and in-Situ Monitoring of Local pH Gradient during Near-Neutral Electrochemical Water Splitting.

Keisuke Obata¹, Roel van de Krol^{1,2}, and Fatwa F. Abdi¹

(1)Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany, (2)Department of Chemistry, Technical University of Berlin, Berlin, Germany

Water splitting in near-neutral pH solutions is attracting significant attention since it offers a path to achieve safe and sustainable (photo)electrochemical hydrogen production. However, the build-up of pH gradients during proton coupled electron transfer reactions is a major concern under pH-neutral

conditions. Understanding the extent of this limitation is, therefore, essential for the design of highly-efficient (photo)electrochemical water splitting systems.

In this study, pH changes during water splitting in a stagnant electrochemical cell are monitored in-situ by a pH-sensitive fluorescence sensor foil placed between the anode and cathode. Our setting clearly shows that electrolyte close to the anode and cathode gets more acidic and more alkaline, respectively, in unbuffered and buffered neutral-pH conditions. A closer look at the pH distribution within the cell further reveals that natural convection is generated by the electrochemical reactions under non-stirred conditions. Specifically, at low current densities ($\leq 2 \text{ mA/cm}^2$), the acidic and alkaline regions move to the top and bottom of the cell, respectively. Based on this observation, we developed a model that considers natural convection driven by buoyancy forces due to local changes in the density of the electrolyte. We found that local pH gradients in the absence of the buoyancy effect are significantly overestimated while the model with buoyancy accurately reproduces the measured pH profile. Overall, the present study clearly reveals the importance of natural convection driven by electrochemical reactions in stagnant solutions. Further implications of our findings for designing efficient (photo)electrochemical water splitting devices will be discussed.

Numerical Modelling of Ceria Undergoing Reduction in a Particle–Gas Counter-Flow: Effects of Chemical Kinetics Under Isothermal Conditions.

Sha Li¹, Vincent M. Wheeler², Apurv Kumar³, and Wojciech Lipiński¹

(1)The Australian National University, Canberra, ACT, Australia, (2)University of Wisconsin, Stout, Menomonie, WI, (3)School of Science, Engineering and Information Technology, Federation University Australia, Mt. Helen, Ballarat, Australia

A numerical model is developed to simulate a single tube reactor featuring a downward particle flow counter to an upward inert gas flow for ceria reduction in the dilute flow regime. The coupled phenomena of mass and momentum transfer as well as chemical kinetics are simulated assuming isothermal operation for the reactor. The model predicts the reduction extent under varying reaction kinetics as well as design and operational choices. It is found that the reduction extent increases with the reaction rate constant until achieving the thermodynamic upper limit at a certain critical value. This critical rate constant signifies a transition from a chemical kinetics limited conversion to a gas advection limited conversion. The effect of reactor length on the reduction extent is through influencing the particle residence time while that of particle size is through impacting both the particle residence time and reaction kinetics. An empirical correlation is developed to quantify the effects of particle and gas flow rates on reduction extent at both slow and fast kinetics. The results offer insights on reactor design and operation towards achieving the maximum reduction extent. Moreover, this numerical work corroborates our thermodynamic model and paves the way for the development of a follow-up two-phase heat transfer model.

Exploring Gradient Functional Material for Enhanced Performance of Solar-Driven Thermochemical Fuel Production.

Da Xu and Meng Lin

Department of Mechanical and Energy Engineering, Southern University of Science and Technology, Shenzhen, China

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Porous material is the key energy conversion media in two-step solar thermochemical fuel production devices. The conventional way of fabricating porous metal oxide structure showed limited tunability in varying local morphology. The recent development of direct ceramic 3D printing technologies enables a unique route for the fabrication of gradient functional materials with complex structures. The triply periodic minimal surface (TPMS) structures are promising candidates due to their flexible lattice structure design, well-defined analytical expression, and easiness in anisotropic feature introduction.

In this study we focus on the characterization and optimization of TPMS structures' multi-physical transport properties for the application in solar thermochemical fuel generators. The TPMS scaffolds are screened in terms of porosity, specific surface area, mean pore diameter, and tortuosity by tuning their governing formula. A comprehensive and flexible modeling framework is developed to evaluate morphological properties, radiative transfer properties, as well as effective mass and heat transfer properties for both experimentally scanned and artificially generated geometries. This advanced structure-property characterization tool is further used for the optimization of TPMS structures under direct solar irradiation for enhanced light absorbing, uniform temperature distribution, favored heat and mass transfer, and increased reaction kinetics. The impact of the optimized TPMS structure material on the device level performance is demonstrated based on a 2D multi-physics model and its comparison with conventional random structure are also shown.

In summary, the quantification of structure-property relationship and the subsequent structure-efficiency relationship offers a promising pathway for the enhanced solar fuel generation based on thermochemical cycles.

KEYNOTE 2

Keynote Talk: Processes for Solar Thermochemical Fuel and Commodity Production.

Martin Roeb

Institute of Solar Research, DLR (German Aerospace Center), Cologne, Germany

Thermochemical and thermo-electrochemical multistep processes can be used to enhance the availability of solar energy in terms of energy transport, of energy demand/supply management and of potential energy carrier related applications. Coupling concentrated sunlight to suitable sequences of thermochemical reaction enables the production of fuels like hydrogen or syngas and other fuels by water- and/or CO₂-splitting as well as the storage of solar energy by breaking and forming chemical bonds in suitable reversible reactions. These processes are sustainable and environmentally attractive since water and CO₂ are used as the only raw materials and solar power and heat as the only energy source. All other materials involved are recycled within the process. The concentrated solar energy is converted into storable and transportable chemicals and fuels. One of the major barriers to technological success of many of those processes is the identification of suitable active materials like catalysts and redox materials exhibiting satisfactory durability, reactivity and efficiencies. Beyond this, solar radiation can be transformed into high temperature heat needed for chemical commodities' production (in endothermic reactions involving inorganic compounds) to provide commodities like cement, lime, phosphate, ammonia, fertilizer, sulfur and sulfuric acid, oxygen, pigments and many more.

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The present contribution investigates how central solar receiver systems can be applied to integrate concentrated solar radiation into high temperature processes forming the basis for production of such kind of products. It will be shown how key components like receivers, reactors, conveying systems and heat exchangers are developed and tested for such applications. In some cases the full production chain from the raw material to the product is demonstrated using a solar facility like a solar tower. Besides materials aspects also process engineering issues needs to be overcome to develop such processes. Challenges are to couple an intermittent energy source to a chemical process and to efficiently recover high temperature heat. The most integration schemes and processes are being described and discussed with respect to further development and future potential.

TECHNICAL SESSION 3: THERMAL ENERGY STORAGE 2

Design Path and Challenges of a Next-Generation, Refractory-Lined, Molten-Salt Storage Tank.

James Yates Jr.¹, Brad Morrison², Gordon Bigham², and Paul Evans¹

(1)Process, Job Industrial Services, Salt Lake City, UT, (2)Mechanical, Job Industrial Services, Salt Lake City, UT

Abstract. Job Industrial Services (JIS), in conjunction with the National Renewable Energy Laboratory (NREL), has performed engineering design and finite element analysis (FEA) of a next-generation, refractory-lined, molten-salt storage tank under the US Department of Energy (DOE) Generation 3 Concentrating Solar Power (CSP) program. The DOE is exploring the use of a new ternary blend of chloride salts (MgCl₂/KCl/NaCl) for thermal energy storage at temperatures significantly higher than the nitrate-based salt used in current CSP plants—720°C versus 565°C. The new salt has increased thermal stability and allows for increased operating temperature, designed to enable use of a more efficient plant power cycle based on the supercritical carbon dioxide Brayton cycle. The design for the storage tank is based upon American Petroleum Institute (API) Standard 650, Welded Steel Tanks for Oil Storage. However, because temperatures are significantly higher than allowed in the API code, the American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel Code (BPVC) and FEA analysis were also used to ensure an adequate and safe design. Although a steel tank with a refractory liner system has significant design challenges, a stand-alone, non-lined tank would involve the use of impractically expensive, high-nickel alloy materials. This work focuses on the FEA design methodology as well as the technical and economic challenges associated with designing a next-generation, refractory-lined storage tank at the brink of the working limits of practical materials.

Long Duration Thermal Energy Storage Using Thermo-Photovoltaics and Solid Storage Media.

Dustin Nizamian^{1,2}, Leah Kuritzky¹, Ben Johnson¹, Tarun Narayan¹, Justin Briggs¹, David Bierman¹, Andrew Ponec¹, and Sean Lubner²

(1)Antora Energy, Berkeley, CA, (2)Lawrence Berkeley National Lab, Berkeley, CA

Thermo-photovoltaics (TPVs) turn photovoltaics into solid-state heat engines that convert heat from a local thermal emitter directly into electricity. By recycling photons of energy below the PV band gap back to the thermal emitter, TPVs can achieve much higher efficiencies than solar PV. TPVs can be used in conjunction with a sensibly heated solid media to realize cheap and scalable long duration thermal energy storage systems. Our team recently broke the world record for solid-state heat engines,

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achieving a thermal-to-electric conversion efficiency greater than 30% using TPVs. Currently, we are investigating optimal properties for thermal energy storage media to help leverage TPV heat engines for thermal energy storage applications.

On the Influence of Spatial Correlations on Radiative Transport in Particulate Media.

Bingjia Li and Rohini Bala Chandran

Mechanical Engineering, University of Michigan, Ann Arbor, MI

Multiphase radiative transport in particulate media has important applications in solar and nuclear energy, additive manufacturing, combustion and chemical catalysis. While the theory of independent scattering is commonly applied to model radiative transport an ensemble of large particles, prior research in this field has shown the limited applicability of such an approach. The goal of this study is to examine the influences of the three-dimensional spatial distributions or spatial correlations of particles in a packed bed on radiative transport. Spatial distributions of the particles were statistically quantified by obtaining an index of clustering using the cubic sampling technique (ICS). Radiation-particle interactions were calculated by performing collision-based Monte Carlo ray tracing simulations. Results indicate that the radiative transport in a packed-bed is strongly correlated to the index of clustering of the particles in the bed. Compared to a Poisson distribution of particles, spatially ordered beds result in lower transmittance and clustered beds resulted in larger values for transmittance, even with the same solid volume fraction. Correlations are obtained to relate the transmittance to the ICS value and the fractions of clusters in fixed beds of particles.

High-Temperature Measurement of Thermophysical Properties of Bulk Material and Coating Using Modulated Photothermal Radiometry.

Jian Zeng¹, Renkun Chen², and Kaman Chung¹

(1)Mechanical and Aerospace Engineering, University of California, San Diego, San Diego, CA, (2)MAE, UC San Diego, La Jolla, CA

We report the instrumentation development of high-temperature thermal conductivity measurement of bulk materials and coatings using a modulated photothermal radiometry (MPR) method. While MPR has been previously established, it has not been well studied for high temperature measurements for bulk and coating materials, both of which are increasingly important for a multitude of applications, especially for materials used in concentrating solar power (CSP) plants. MPR is a non-contact technique and utilizes intrinsic thermal emission from the specimens for thermometry, which is favorable for the measurement at high temperature in harsh environment. We design and utilize sample holders especially for the high temperature measurement up to 1000 K with a good temperature uniformity within the sample. The high-temperature MPR setup is validated by measuring bulk materials with known thermal conductivity and the measurement uncertainty is less than 10%. We then extend the technique to measure black solar-absorbing coatings of 10 to 50 μm thick on various substrates by modulating the frequency of the heating laser beam and the thermal penetration depth. We show that thermal conductivities of typical solar absorbing coatings are $0.4 \sim 0.8 \text{ W m}^{-1} \text{ K}^{-1}$, indicating a possibly large temperature drop within the coating under high solar irradiation flux condition, such as over 1000-sun for central solar towers.

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Thermal Radiative Property Measurements of Particulate Media.

Mike Mayer and Rohini Bala Chandran

Mechanical Engineering, University of Michigan, Ann Arbor, MI

Next-generation concentrated solar power (CSP) technology relies on higher temperatures to reach higher efficiencies, but this requires a heat transfer medium that can withstand these elevated temperatures (~1000°C). One potential pathway that has been identified for cost-competitive CSP is the falling-particle receiver which utilizes solid particles, such as sand or other ceramic materials, as the heat transfer and storage medium. Effective particles for this application have high solar absorptance while minimizing thermal emittance in the temperature and spectral ranges encountered in a solar receiver. Optical property data for these materials can be crucial in determining their usefulness in a CSP application. However, data for many of these ceramic materials, and combinations thereof, is not readily available or reliable, especially at elevated temperatures. One method for measuring optical properties with high resolution is Fourier transform infrared spectroscopy. In the case of a powdered material, this technique can be used to measure diffuse spectral reflectance by diluting the sample with an IR transparent matrix and placing that mixture into a DRIFTS accessory. This collects the diffuse reflections and directs them to the detector of the FTIR. Results are reported at room-temperature for CARBO Accucast ceramic proppants, one candidate for falling-particle receivers. Additional (spectral) measurements are planned at higher temperatures for both diffuse reflectance and emittance using an environmental chamber and thermal stage coupled with collimating optics, respectively.

TECHNICAL SESSION 4: SOLAR FUELS & THERMOCHEMICAL ENERGY STORAGE

Invited Talk: Future Directions and Challenges for Solar Thermochemical Energy Storage.

Nick AuYeung¹, Fuqiong Lei¹, Alexander Dyll¹, and Lucas Freiberg²

(1)School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, OR,

(2)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR

Solar thermochemical energy storage has great promise but also great challenges. Presented here will be some perspectives on the complexities of integrating thermochemical storage into CSP. The focus of the TCES community is now on redox reactions. Important advances in the field as well as our recent work to improve barium peroxide based materials will be discussed. As a community, we need not only better materials but more cost-effective storage systems. The storage duration at which solar TCES provides a winning value proposition over sensible energy storage remains to be defined. Integration into chemical processing may provide another potential application for TCES.

Invited Talk: Materials Thermodynamic Limits in Solar-Thermochemical Fuel Production

Ivan Ermanoski, James E. Miller, and Ellen B. Stechel*
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Solar-thermochemical (STC) carbon dioxide and water splitting is a pathway for the direct thermal production of solar fuels—an alternative to direct thermolysis. Currently, the most widely researched implementation is the two-step cycle. Reducing two-step cycles to practice is challenging, and there is a substantial ongoing effort to improve reactor designs, and to synthesize redox active materials that exceed the STC potential of ceria, the current state-of-the-art redox active material. We have analyzed the underlying general thermodynamic boundaries that lead to materials performance tradeoffs between heat of reduction, productivity, and yield. These boundaries apply to all nonstoichiometric oxides without phase changes during redox cycles, or where the phase changes are energetically negligible. We quantify the tradeoffs between the desirable decrease of the heat of reduction and penalties such as decreasing yields and increasing cycling temperature range, and show that operating parameters pose firm limitations on cycle performance and on the desirable materials properties space.

The Thermodynamics of Magnesium Manganate Reduction for Application in Thermochemical Energy Storage Systems.

*Jayni Hashimoto, Srashtasrita Das, Harsheen Rajput, and Christopher L. Muhich
Chemical Engineering, Arizona State University, Tempe, AZ*

Thermochemical energy storage shows potential for providing energy for a full 24 day when combined with solar power plants and conventional electricity production means. Operating the system at high temperatures allow for high levels of efficiency to be reached, and the long-duration ability of the technology allows for this type of storage to be used to replace current systems, or to supplement existing infrastructure. MgMn_2O_4 is of interest as they are low cost and have high reduction/oxidation temperatures. The storage capacity of any potential system is determined by the energy density of the material; therefore we report on the energy density of this material as well as its underlying thermodynamics, using Van't Hoff analysis in conjunction with thermogravimetric data. Density functional theory calculations are used to understand the thermodynamic limitations. We explore the material as a function of Mg:Mn content, and provide novel means of increasing the reactivity. Additionally, material characterization confirms the phase purity of the synthesized material.

Thermal Reduction of Iron-Manganese Oxide Particles in a High-Temperature Packed-Bed Reactor for Solar Thermochemical Energy Storage.

Bo Wang¹, Lifeng Li¹, Florian Schäfer², Johannes J. Pottas¹, Apurv Kumar³, Vincent M. Wheeler⁴, and Wojciech Lipiński¹

(1)The Australian National University, Canberra, ACT, Australia, (2)ETH Zurich, Zurich, Switzerland, (3)School of Science, Engineering and Information Technology, Federation University Australia, Mt. Helen, Ballarat, Australia, (4)University of Wisconsin-Stout, Menomonie, WI

The reduction of iron–manganese oxide particles in a high-temperature packed-bed solar thermochemical reactor is investigated using an advanced transient three-dimensional computational fluid dynamics model. By coupling the conductive, convective, and radiative heat transfer, reaction kinetics, and fluid flow, the model offers a detailed description of the transport phenomena in the indirectly irradiated packed bed. A reactor prototype that features a reaction tube confining the packed particles and a surrounding cavity is tested under simulated high-flux solar irradiation to validate the

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model. The numerically predicted temperature profiles and oxygen generation rates are in good agreement with the experimental data. The validated model is used to evaluate the performance of the reactor. For the baseline case, the calculated temperature profiles indicate that the non-uniform temperature distribution in the start-up phase is later homogenized by the thermal emission of the reactor components at elevated temperatures. When the reaction takes place, the maximum temperature difference in the reactive zone is less than 100 K. An energy rate balance analysis shows that the instantaneous peak solar-to-chemical energy efficiency reaches 9.3%. The sensible heat reservoir is the primary cause of heat loss. The peak solar-to-chemical efficiency rises to 11.36% after optimizing the batch-mode operating conditions. Under the optimal operating conditions, the particles are processed at a mass flow rate of 1.44 mg s^{-1} . The reaction extent of each batch is 95.5%.

KEYNOTE 3

Keynote Talk: Materials, Reactors and Systems for Efficient and Scalable Production of Solar Fuels Using Thermochemical Cycles.

Ahmed F. Ghoniem¹, Aniket Patankar¹, Wonjae Choi², and Xiaoyu Wu¹

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Solar Fuels offer a promising route for deep decarbonization by enabling large-scale, long-term storage of renewable energy, and directly replacing fossil fuels in industry and transportation. In research, we adopt a multi-scale approach for realizing efficient and scalable production of solar fuels via two-step thermochemical cycles using metal oxides. At the micro-scale we focus on material design with high oxygen carrying capacity and fast kinetics. At larger length scales, we work on reactor designs with emphasis on solid heat recovery in temperature-swing thermochemical cycles. Finally, we examine strategies for system integration to achieve efficiency and co-generation. In this talk, we will review recent progress, and share relevant past and current research at the Reacting Gas Dynamics Laboratory at MIT. We conclude by reflecting on the economic prospects of thermochemical solar fuel production and highlighting the need for accelerated research and development in the area.

TECHNICAL SESSION 5: PROCESS, SYSTEMS AND MATERIALS MODELING

Optical Analysis of a Novel Solar Thermochemical System with a Rotating Tower Reflector and a Receiver–Reactor Array.

Lifeng Li¹, Song Yang², Bo Wang¹, John Pye¹, and Wojciech Lipiński¹

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We propose a novel concept of a rotating tower reflector (TR) in a beam-down optical system to alternate concentrated solar irradiation of an array of solar receiver–reactors, realizing multi-step solar thermochemical redox cycles. Heat recovery can be implemented in the receiver–reactor array, which is reported to result in dramatically improved thermal-to-chemical efficiency of receiver–reactors from 3.5% to 20%. Here, optical and radiative characteristics of the proposed optical system are explored analytically and numerically by Monte-Carlo ray-tracing simulations.

ORAL ABSTRACTS

We identify the optimal geometrical parameters that offer the maximum system optical efficiency. A baseline system is found to provide a solar concentration ratio of 2588 suns with an instantaneous system optical efficiency and radiative power to the receiver–reactor of 51% and 16 MW, respectively. TR axis is required to be tilted for accommodating the receiver–reactor array, resulting in reduced optical efficiency. We demonstrate that the annual optical efficiency of a baseline system with the receiver–reactor located south of the tower decreases from 46% to 37% for the axis tilt angle of TR increasing from 2° to 20°. Locating the receiver–reactor array south of and as close as possible to the tower offers the most promising optical configuration. The optical analysis conducted in this study provides a general formulation to enable predictions of thermal-to-chemical efficiency of the receiver–reactor array and overall solar-to-chemical efficiency of the solar thermochemical plant.

Unified Design Guidelines for High Flux Solar Simulator with Controllable Flux Vector.

Jieyang Li¹ and Meng Lin²

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High-flux solar simulator is an essential tool in the field of concentrated solar applications creating stable and controllable irradiation environments with flux magnitude and spectrum close to really solar concentrators. This feature enables reliable characterization of thermochemical materials, reactor/receiver designs, and solar conversion systems via artificially generated stable condition ruling out the effects of unstable real solar irradiation. A broader utilization of HFSS requires flexibility in controllable flux magnitude (concentrated or uniform) and incidence angle distribution (directed or random).

In this study, we provide a comprehensive investigation for the design of HFSS with controllable magnitude and distribution (spatial and angular) based on Monte Carlo Ray Tracing techniques. A combined uniformity index is proposed considering the global standard deviation, radial homogeneity, and axial homogeneity. The statistic histogram of incidence angle distribution at the focal plane is used to extract angular information. The effects of eccentricity of the reflector, off-focus of lamp, reflector truncation, reflector position, off-focus of target, as well as adding CPC and homogenizer on the final flux vector are presented. Higher eccentricity leads to a smaller peak flux. There is an optimal lamp position relative to the reflector's focal point. Moving the lamp out of focal point in radial direction for 3 mm leads to a peak concentration increase by 42.21%. Non-central lamp units help increase the uniformity. Adding CPC or homogenizer can further tune the angular and flux distribution enabling potential for various solar conversion applications.

Sorption Pumping of O₂ Pumping Using Alpo-5 Zeolites: A Density Functional Theory Study.

Steven Wilson

Chemical Engineering, Arizona State University, Tempe, AZ

Solar thermochemical fuel generation via chemical looping of metal oxides has the potential for high solar conversion efficiencies. Operating at temperatures less than 2000C, requires oxygen partial

pressures to be maintained as low as possible, ($P_{O_2} < 100\text{Pa}$). This has conventionally been provided by mechanical pumping or the use of an inert sweep gas. Both methods are a major source of energy loss in the system. Sorption pumps are a novel means to mitigate this loss. Zeolites offer a high surface area of adsorption without the need for oxygen to diffuse through any crystal lattice. In the proposed system, O_2 is adsorbed at room temperature, then using readily available waste thermal heat, the zeolite temperature is raised driving off the O_2 and regenerating the pumping capacity. In this work, we use *ab initio* calculations to demonstrate the feasibility of using Zeolites for oxygen pumping. Our calculations indicate that selective doping of Pt into the Tetrapropylammonium Hydroxide (ALPO-5) zeolite provides six unique sites for O_2 chemical adsorption in a desired 40-60 kJ/mol regime. Two of the six sites have a negative adsorption energy of -55.7 and -88.2 kJ/mol. The success of doping with Pt indicates that other, less expensive dopants maybe found. We have identified two additional suitable dopants. This initial investigation encourages future research and application and demonstrates the feasibility of this technology. This will provide a new, low energy cost method for oxygen pumping, overcoming one of the key energy inefficiencies in the overall solar to fuel conversion.

Optimal Selection of Ions for Perovskite Solar Cell Synthesis through a Computational Approach.

Swapana S. Jerpoth¹, Joseph Iannello², Emmanuel A. Aboagye¹, and Kirti M. Yenkie¹

(1)Chemical Engineering, Rowan University, Glassboro, NJ, (2)Mechanical Engineering, Rowan University, Glassboro, NJ

Perovskite solar cells have gained tremendous attention in recent years due to continued enhancement in their performance efficiency. However, the long-term stability of the device has been a major drawback that has prevented its global commercialization. To overcome this challenge the synthesis mechanism and the materials involved need to be further improved for better stability and high efficiency at optimum costs. Hence computational modeling and predictions can play a significant role in finding new functional materials. Perovskites are defined with the stoichiometry of ABX_3 , where A, B are cations and X is an anion. To determine the formability of perovskites, two important factors (octahedral and tolerance) described by Goldschmidt play a vital role. We propose an integrated methodology that can select an optimum combination of different ions for the perovskite solar cell, based on the Goldschmidt stability factors, and simultaneously minimize the material cost. The mathematical formulation is an optimization problem with the objective as minimization of the total costs and the constraints being the tolerance factors and the structural parameters. The ions for the respective sites in the perovskite crystal are selected using binary integer decision variables, while the cost leads to a linear function; hence the overall problem is a mixed-integer linear programming problem. Programming tools in MATLAB and GAMS are used for solving the problem. The results indicate that the optimal perovskite crystal structure is ammonium-magnesium-formate with a cost of 0.18 (\$/g) while the percentage variation in cost from the first-best combination to the second-best is 19.2%

Semi-Automatic Method to Optimize Multi-Lamp High Flux Solar Simulators Utilizing Machine Learning Algorithms.

Konstantinos E. Kakosimos¹, Daniel Haseler², and Arshad Mohamed Ali³

(1)Texas A&M University at Qatar, Doha, Qatar, (2)Electrical Engineering, Texas A&M Univeristy, College Station, TX, (3)Chemical Engineering, Texas A&M University at Qatar, Doha, Qatar

ORAL ABSTRACTS

Extensive research is being conducted on photon energy driven reactions which include wastewater treatment, H₂ production, and advanced material aging under diffuse or concentrated light. Solar simulators are a convenient tool for the latter research applications because they allow emulation of solar radiation under well controlled laboratory conditions. Most concentrated light simulators are comprised by multiple light sources with ellipsoidal or parabolic mirrors. Thus, they require accurate characterization of various system parameters such as peak flux and flux density distribution. At the same time, they also require optimization to ensure system can operate at its theoretical maximum flux and provide the necessary radiating energy. However, this process is either manual or semi-automated and demands expert-user intervention – i.e. a tedious and time consuming process. This study utilizes the High Flux Solar Simulator (HFSS) facility at Texas A&M University and presents an automated system for the characterization of the irradiance, collection of experimental data, and most importantly control of the irradiance. At first, irradiance was characterized by using the flux mapping method. Then, the data were used to train a semi-supervised machine learning algorithm based on a typical convolutional neural network model. Finally, the model was used to optimize alignment of the light sources (three degrees of freedom per source) given variable flux parameters i.e. peak flux and flux distribution. The proposed methodology is expected to facilitate initial deployment of high flux solar simulators and assist on the dynamic control of reactor conditions i.e. emulating variable overcast or daily sunlight variability.

Using Monte Carlo Ray Tracing and Data-Driven Techniques for Radiative Transport in Particulate Media.

Zijie Chen and Rohini Bala Chandran

Mechanical Engineering, University of Michigan, Ann Arbor, MI

Radiative energy transport in particulate media including packed-beds, granular flows and fluidized beds plays a crucial role in concentrated solar power. To fully resolve radiative energy transport in multiphase media, the challenge is to compute absorption, emission and scattering of photons through the medium. Here, we develop and apply the Monte Carlo ray tracing to track the path and intersection points of numerous rays or energy bundles to determine view factors between pairs of particles and surfaces. View factor quantifies the fraction of radiative energy directly intercepted by a surface, and hence for N-particles system in a packed-bed, the calculation of view factors by tracing $\sim 10^6$ rays presents a huge computational challenge. To lower computational cost, we propose to use the physics-based predictions of view factors to inform the development of data-driven correlations using techniques like least-square regression. These predictions resulted in view-factor correlations that depended only on geometric parameters including the ratio of the inter-particle distance to the particle diameter and the particle-bed solid volume fraction. Results for the particle-to-particle view factors show three distinct regimes with respect to dimensionless distance — a monotonic decay regime, a shading-dominated regime and a large-distance regime with negligibly small view factor values. For the shading-dominated regime, physical laws of shading are applied to simplify the view-factor prediction. The techniques developed here to obtain geometry-dependent view-factor correlations are anticipated to be more computationally tractable to evaluate radiative heat transfer, especially in systems with large numbers of particles and multiphase flows with moving particles.

TECHNICAL SESSION 6: SOLAR PROCESS HEAT/ WATER TREATMENT

Invited Talk: Efficient Utilization of Solar Energy for Wastewater Treatment *Via* Radiative Heating.

Akanksha Menon¹, Robert Kostecki², and Ravi Prasher³

(1)Energy Technologies Area, Lawrence Berkeley National Lab, Berkeley, CA, (2)Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, Berkeley, CA, (3)Energy Technologies Area, Lawrence Berkeley National Laboratory, Berkeley, CA

Global demand for water is projected to increase by 55% by 2050, and this has brought the treatment of non-traditional water sources, *i.e.*, desalination to the forefront. Of particular interest for the water-energy nexus is the integration of desalination technologies with renewable sources such as solar energy. For instance, evaporation ponds harness solar energy to passively evaporate water from brines to achieve zero-liquid discharge (ZLD). However, direct utilization of solar energy for evaporation is limited by the transparency of water at visible and near-infrared wavelengths. To address this, we demonstrate a simple photo-thermal device that converts sunlight into mid-infrared radiation where water is inherently a strong absorber. This causes radiative heat localization at the water's surface, resulting in over a two-fold enhancement in evaporation at a solar-thermal efficiency of 43%. Furthermore, the non-contact nature of radiative heating eliminates contamination risks, thus making the device uniquely suited for passive wastewater management. Photo-thermal converters can also be applied to desalination of oil and gas produced water using forward osmosis (FO), in which a draw solution drives water flux across a membrane. However, separation of the draw from water, *i.e.*, regeneration presents an energy bottleneck. To address this, we use a novel class of thermally responsive draw solutes that can be regenerated using solar heat for clean water production. Here, a photo-thermal converter delivers infrared emission overlapping with the absorption spectrum of the water-draw mixture to induce phase separation *via* radiative heating. This serves as an ideal candidate for energy-efficient and low-cost desalination.

Invited Talk: Techno-economic Analysis of SCEPTRE™ – Solar Cascading Evaporation Process to Recover Effluent.

Brandon Hathaway

Sunvapor Inc., Pasadena, CA

The conventional method of high-water recovery brine treatment is based on mechanical vapor recompression (MVR). MVR has serious drawbacks: (1) high electricity consumption, (2) high capital and maintenance costs, and (3) reliance on baseload electricity generated from fossil fuel. Addressing the fossil fuel consumption problem using solar thermal energy is possible through thermal vapor recompression (TVR) technology by replacing the MVR compressors with thermal vapor compressors powered by motive solar steam. The energetic and cost challenges remain, however. When using thermal energy input, energy consumption increases significantly, and the need for waste heat rejection becomes significant. Economically, high capital costs of the TVR and heat rejection systems combined with inherently low utilization due to the intermittent nature of solar power results in prohibitively high costs of brine recovery. Overall, this conventional solar approach lacks a competitive edge, preventing commercial adoption.

ORAL ABSTRACTS

To overcome the disadvantages of conventional high recovery processes like MVR or limitations of solar thermal implementations utilizing TVR, Sunvapor has invented a process, Solar Cascading Evaporation Process to Recover Effluent (“SCEPTRE™”) that utilizes moderate temperature waste heat to nearly double the efficiency of thermal brine concentration while reducing the size of the most capital-intensive unit processes, thereby offering a path to lowering the cost of water produced by incumbent grid-connected mechanical vapor recompression while utilizing primarily solar thermal input. In this paper, we present a Technoeconomic Analysis of this process.

Lost Hills Solar - Powering an Oil and Gas Field with Renewable Energy.

Trevor Demayo

Chevron, Bakersfield, CA

In an effort to reduce greenhouse gas emissions and manage energy costs, Chevron’s San Joaquin Valley Business Unit decided to build a solar photovoltaic plant to offset grid power consumption in its Lost Hills oil and gas field. A 29 MWAC, 220 acre solar plant was designed to power the field during the day and sell excess power to the grid to help offset night-time electricity purchases. It is expected to provide more than 1.4 billion kilowatt hours of clean solar energy over 20 years to the field’s production and processing facilities, meeting approximately 80 percent of the field’s energy needs. In addition to the solar array, the project also included upgrading utility transmission lines and the field’s substation, which included new technology to reduce the risk of sulfur hexafluoride emissions, another potent greenhouse gas. The solar plant, commissioned in April 2020, operates under a Power Purchase Agreement with the solar PV provider and will generate California Low Carbon Fuel Standard credits as well as federal Renewable Energy Certificates. This talk will describe the journey and challenges by a major oil and gas company to build one of the first net exporting, behind the meter solar PV plants in California.

Effects of Competing Reactions and Effluent Stream Composition on the Energy Efficiency of a Photoelectrochemical Wastewater Nitrate Treatment Device.

Luisa Barrera and Rohini Bala Chandran

Mechanical Engineering, University of Michigan, Ann Arbor, MI

Nitrates are present in industrial effluent streams from fertilizer production, iron/steel making and finishing, coal mining, and municipal wastewater streams. Typically, nitrates are eliminated from wastewater through biological nitrification-denitrification treatment processes, but these are energy intensive and can only be used for wastewater streams in which microbial growth is suitable. In prior work, we’ve discussed a solar-powered photoelectrochemical device to treat wastewater nitrates, concluding that the formation of ammonia and nitrous oxide allowed for additional energy recovery as compared to the common electrochemical denitrification approach that transforms nitrates into nitrogen. In this study, an equivalent circuit and kinetic model was developed to specifically investigate the influences of competing redox reactions and the effluent stream nitrate concentration on the overall energy performance of this device. Competing reactions of interest were hydrogen evolution reaction, hydrogen oxidation reaction, oxygen reduction reaction, in addition to possible side-reactions of the formed nitrogen-species. Model results indicate that the extent at which the cathodic side reactions compete with the nitrate reduction reaction depends on the nitrate concentration present in the waste

ORAL ABSTRACTS

stream, the electrocatalytic parameters of the reactions, and the band gap of the light-absorber. It was also found that the oxygen reduction reaction has a significant effect on the overall solar energy conversion efficiency and energy consumption of the considered device. Overall, the energy consumption of the proposed device is comparable to current ammonia and nitrous oxide formation processes, with the additional benefit of recovering nutrients and using a renewable energy source.

Modeling of a Hybrid Membrane Distillation/ Photovoltaic Cell.

Alejandro Espejo Sanchez

Boise State University, Boise, ID

Membrane distillation (MD) for high salinity water treatment can be combined with renewable energies. A hybrid system capable of absorbing energy for the temperature requirements and generating electricity is developed by integrating a membrane for water desalination and a photovoltaic (PV) cell to generate electricity. At the top of the system is a photovoltaic cell which filters the visible light wavelengths and transmit the remaining ultraviolet and infrared to a membrane doped with absorbing nanoparticles located at the core of the system. A mass and heat transfer model of this hybrid design is developed to accurately replicate the system performance. The physical and solar properties of the photovoltaic cells, membranes, and direct contact membrane distillation (DCMD) setup are incorporated into the model. The model develops the parametric equations that characterize the generation of electricity and clean water. The design parametric is capable to determine the effect of different photovoltaic cells, nanoparticle-doped membranes, flow rates, and flow temperatures. This study provides a new method to predict the photovoltaic electric flux, membrane temperatures, and membrane water flux.

Modelling a Conveyor-Belt Solar Receiver to Dry and Heat Aggregates in Hot Mix Asphalt Industry.

Dario Pardillos Pobo¹, Jesus Gomez Hernandez², and Todd Otanicar³

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(3)Mechanical and Biomedical Engineering, Boise State University, Boise, ID

A new solar receiver is proposed to dry aggregates in Hot Mix Asphalt (HMA) production, to reduce the current consumption of $136 \cdot 10^6$ MWh/year of fossil fuels and the associated greenhouse gases emissions. The solar receiver is coupled to a linear beam-down solar field, which employs two reflections to redirect the solar irradiation towards the ground, where the solar receiver is placed. The solar irradiation is concentrated on the surface layer of particles, which are transported using a conveyor belt.

The particles drying and heating processes are modelled by an iterative procedure to solve the energy balance equations at steady state for each time period. An explicit finite difference method is used to calculate the particles temperature evolution position.

An industrial conveyor belt solar receiver has been simulated, with a width of 1 m, a total length of 300 m and a particle layer thickness of 0.04 m. The production is estimated in 300 tons/day, the usual of an HMA plant. To deal with punctual demand, the hot particles are stored in an adiabatic tank. The installation, which includes a 5100 m^2 solar field, produces HMA with a cost of 0.41 \$/ton.

ORAL ABSTRACTS

Concentrating solar technology for process heating is an interesting way to dry and heat particles, while fighting against climate change. Further simulations will focus on water diffusivity in aggregates and will compare this concentrating solar technology with conventional fueled processes. In addition, a prototype will be constructed to validate the thermal model.

Technical Potential and Environmental Impact Assessment of PV Electric Powered Industrial Process Heating.

Jingyi Zhang¹, Carrie Schoeneberger¹, Colin McMillan², Parthiv Kurup³, William Xi³, Robert Margolis³, and Eric Masanet¹

(1)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, (2)Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO, (3)National Renewable Energy Laboratory, Golden, CO

Industrial process heating (IPH) takes up 50% of industrial manufacturing energy consumption, and about 90% of IPH is powered by fossil fuel. The combustion of fossil fuel causes great environmental concerns due to the toxic chemicals emitted to the environment. To reduce the environmental impacts, renewable energy is developed to partially replace conventional fossil fuel. PV technology is projected to be applied to different fields due to continuously increasing capacity and decreasing cost. By using PV electric instead of fossil fuel powered IPH in different industrial sectors, the technical potential and environmental impact variations are investigated.

The unit processes in different industrial sectors that can use PV electro-technologies are identified, and the technical potential is estimated from conventional energy consumption with different end uses and technical replacement potential by using PV electro-technologies. Two electro-technologies - electric boiler and waste heat recovery heat pump (WHRHP) that have relatively high potential have been identified, and the CO₂ emission reductions are calculated based on two scenarios: (1) PV technology can fully supply the energy demand by either electric boilers or WHRHPs; (2) based on the land availability in different states, the energy generated from PV can partially or fully supply the energy demand from electric boilers or WHRHP.

From the analysis, it shows that large CO₂ emission reduction can be achieved by replacing conventional fossil fuel based technologies with PV electro-technologies and the results can provide insightful information to stakeholders and policy makers.

Solar Industrial Process Heating: A Technical Potential Analysis for U.S. Manufacturing.

Carrie Schoeneberger¹, Jingyi Zhang¹, Colin McMillan², Parthiv Kurup³, William Xi³, Robert Margolis³, and Eric Masanet^{1,4}

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Clean energy transitions are essential for addressing global sustainability challenges, and a critical target for renewable energy integration is the industrial sector since it has the highest energy consumption of all major sectors worldwide. In the U.S., the vast majority of energy use in the industrial sector is

ORAL ABSTRACTS

associated with industrial process heat (IPH), which relies predominantly on the combustion of fossil fuels, such as natural gas, coal, and oil, to meet process heat energy demand.

With the emergence of increasingly cost-effective and efficient solar technologies, solar industrial process heat (SIPH) is gaining renewed attention as an alternative method for industrial heat production. A broad range of solar thermal and electric heating technologies can be used for process heating, and our work provides analyses that assess these technologies and their technical potential in U.S. manufacturing industries.

This national analysis specifically evaluates the thermal energy demand of IPH that can be provided by a collection of solar technologies, for all regions in the U.S., at an hourly basis, and with consideration of thermal energy storage. Process-level models are integrated with national manufacturing energy use and technical equipment data and are combined with solar energy resource modeling to calculate achievable fossil fuel savings and technical potential on a spatial temporal scale.

We also identify barriers, both technical and economic, that must be overcome to promote future SIPH adoption, and suggest a research agenda for addressing those barriers moving forward.

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ZOOM BACKGROUNDS



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CODE OF CONDUCT

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