



**GORDON RESEARCH CONFERENCES
FINAL PROGRESS REPORT
Department of Energy (DOE)
Grant Number DE-SC0023644
Inorganic Reaction Mechanisms GRC/GRS**

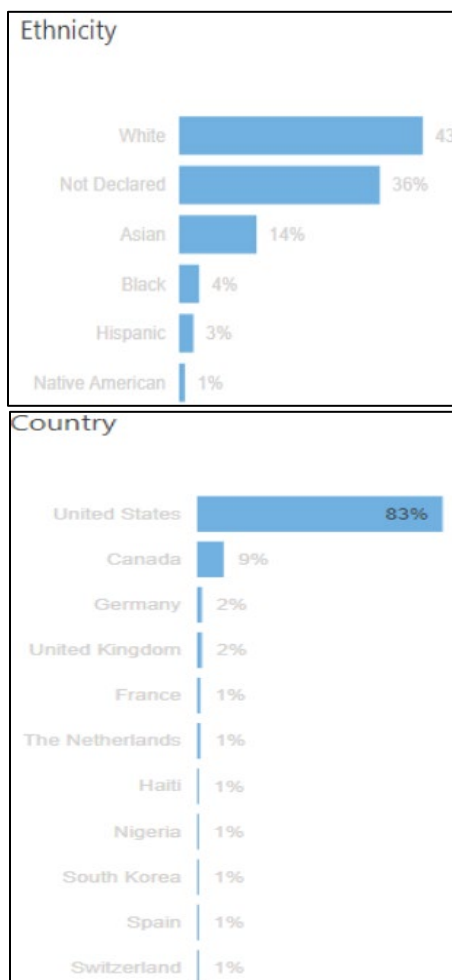
Operational Summary

The Gordon Research Conference (GRC) and Gordon Research Seminar (GRS) on Inorganic Reaction Mechanisms were held at the Grand Galvez in Galveston, Texas from March 5 - 10, 2023. The meeting covered a variety of scientific topics and the content presented was highly rated by participants.



Conference Participants

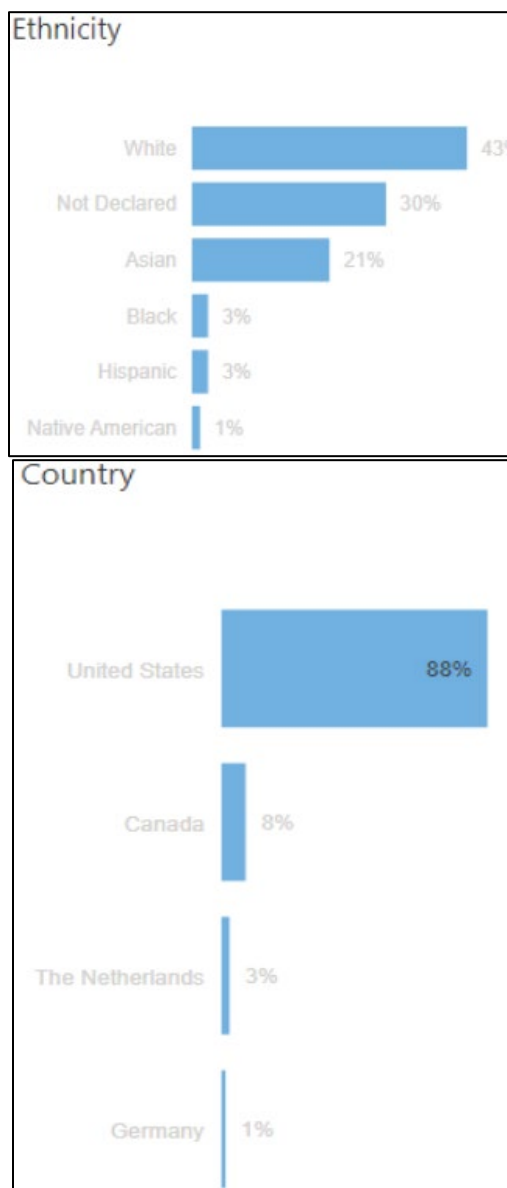
The Conference was well-attended with 154 participants. Scientists from academia represented 85% of the participants while attendees from government accounted for 3%, attendees from industry totaled 6% and those from academic/industrial accounted for 6%. The meeting also attracted a strong mix of young investigators and senior scientists. Students and post-docs accounted for 44% of all attendees. Approximately 30% of the participants at the 2023 meeting were women, 68% male and 1% non-binary. The meeting brought in 91 First Time attendees (48%).



Seminar Participants

The Seminar was well-attended with 61 participants. Scientists from academia represented 85% of the participants while attendees from government accounted for 3%, attendees from industry totaled 7% and those from academic/industrial accounted for 5%. The meeting also attracted a strong mix of young investigators and senior

scientists. Students and post-docs accounted for 88% of all attendees. The remaining attendees served as key mentors during the program and networking opportunities. Approximately 41% of the participants at the 2023 meeting were women and 59% male. The seminar registered that 54 of the 61 participants were first time attendees.



Conference Program

The Inorganic Reaction Mechanisms GRC was a premier, international scientific conference focused on advancing the frontiers of science through the presentation of cutting-edge and unpublished research, prioritizing time for discussion after each talk and fostering informal interactions among scientists of all career stages. The conference program included a diverse range of speakers and discussion leaders from institutions and organizations worldwide, concentrating on the latest developments in the field. The conference was five days long and held in a remote location to increase the sense of camaraderie and create scientific communities, with lasting collaborations and friendships. In addition to premier talks, the conference had designated time for poster sessions from individuals of all career stages, and afternoon free time and communal meals allowed for informal networking opportunities with leaders in the field. The 2023 Inorganic Reaction Mechanisms Gordon Conference covered the spectrum of activities in mechanistic inorganic chemistry, including new mechanistic techniques. The program featured leading scientists from across the field of inorganic chemistry (broadly defined) and also

featured poster sessions open to all attendees. An opportunity was provided for selected poster presenters to give short oral presentations about their work.

The Inorganic Reaction Mechanisms GRS provided a unique forum for young doctoral and post-doctoral researchers to present their work, discuss new methods, cutting edge ideas, and pre-published data, as well as to build collaborative relationships with their peers. Experienced mentors and trainee moderators facilitated active participation in scientific discussion to allow all attendees to be engaged participants rather than spectators. The 2023 GRS featured next-generation approaches and advancements in the study of reaction mechanisms for bio-inorganic, organometallic, inorganic, and materials science disciplines using complementary in-situ and operando spectroscopic techniques. The GRS promoted interactions between the participants and the leaders from academia, national laboratories, and industry, through mentorship and career development programs. In particular, the GRS provided opportunities to debate challenges at the forefront of chemistry.

Conference Budget

Funding provided by the DOE supported registration support for 2 graduate students, 1 post-doc, 3 research scientist/engineers, 4 assistant professors and 3 associate professors at the GRC. The funds supported 2 students, 1 associate professor, 3 research scientist/engineers and 3 post-docs at the GRS. All participants supported were US based affiliates as required.

Conference Feedback

Participants had an opportunity to provide feedback at the end of the Conference. The feedback collected from the meeting was extremely positive. Evaluations included numerous positive remarks regarding the networking opportunities, the interactive poster sessions and the scientific content. The evaluations also included comments about the engaging poster sessions and the quality discussion.

GRC would like to thank the DOE for its continued support of the meetings. The contributions received from the DOE have been critical to the success of the conferences and are having a measurable impact in advancing the frontiers of science worldwide.

Investigators:

Dr. Jennifer A Love, GRC Chair
University of Calgary, Canada

Dr. Elon A Ison, GRC Vice Chair
North Carolina State University, United States

AOR:

Dr. Nancy Ryan Gray, President and Chief Executive Officer
Gordon Research Conferences

Inorganic Reaction Mechanisms

Gordon Research Conference

How Understanding Reaction Mechanisms Transforms Approaches to Solving Challenges in the 21st Century

March 5 - 10, 2023

Chair Jennifer A. Love

Vice Chair Elon A. Ison

Grand Galvez

2024 Seawall Boulevard

Galveston, Texas, United States

Conference Program

Sunday

2:00 pm - 9:00 pm	Arrival and Check-in
6:00 pm - 7:00 pm	Dinner
7:30 pm - 7:40 pm	Introductory Comments by GRC Staff / Welcome and Introduction from the Chairs
7:40 pm - 9:30 pm	Bioinorganic Chemistry Discussion Leader: Elon Ison (North Carolina State University, United States)
7:40 pm - 7:45 pm	Introduction by Discussion Leader
7:45 pm - 8:15 pm	Wonwoo Nam (Ewha Womans University, South Korea) "Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation and Formation Reactions"
8:15 pm - 8:30 pm	Discussion
8:30 pm - 9:00 pm	Eva Nichols (University of British Columbia, Canada) "Mechanistic Insights into Electrochemical CO ₂ Reduction <i>via</i> Second Sphere Modification"
9:00 pm - 9:15 pm	Discussion
9:15 pm - 9:30 pm	General Discussion

Monday

7:30 am - 8:30 am	Breakfast
8:30 am - 9:00 am	Group Photo
9:00 am - 12:30 pm	In Situ and New Methods Discussion Leader: Ethan Crumlin (LBNL, United States)
9:00 am - 9:30 am	Robert Gilliard (Massachusetts Institute of Technology, United States) "Unusual Boron-Doped Heterocycles: Synthesis, Structure, and Mechanistic Insight"
9:30 am - 9:45 am	Discussion

9:45 am - 10:15 am	Coffee Break
10:15 am - 10:45 am	Renee Sifri (Merck, United States) "Application of Transition Metal Catalysis to Pharmaceutical Intermediates at Merck"
10:45 am - 11:00 am	Discussion
11:00 am - 11:30 am	Scott McIndoe (University of Victoria, Canada) "Continuous Addition Kinetic Elucidation: Catalyst and Reactant Order, Rate Constant, and Poisoning from a Single Experiment"
11:30 am - 11:45 am	Discussion
11:45 am - 12:15 pm	Michael Zdilla (Temple University, United States) "Electronic Structure Basis for Water Oxidation in Mineral Chydoloxides: A New Role for the Catalytically Active egl Electronic State"
12:15 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
3:00 pm - 4:00 pm	The GRC Power Hour™ <i>The GRC Power Hour™ is designed to address diversity and inclusion in the scientific workplace by providing a safe environment for informal and meaningful conversations amongst colleagues of all career stages. The program supports the professional growth of all members of our communities, including ethnicity, race and/or gender identity by providing an open forum for discussion and mentoring. Organizers: Lucie Nurdin (Terraform Industries, United States) and Marcus Drover (The University of Windsor, Canada)</i>
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Ligand Non-Innocence: Redox Active/M-L Cooperativity Discussion Leader: Tianning Diao (New York University, United States)
7:30 pm - 8:00 pm	Karen Goldberg (University of Pennsylvania, United States) "Ligand Non-Innocence: Effect on Reaction Mechanism"
8:00 pm - 8:15 pm	Discussion
8:15 pm - 8:45 pm	Kensha Clark (University of Mississippi, United States) "A Hop, Skip, and a Jump: Enabling Rapid Electron Transfer for Multielectron Transformations"
8:45 pm - 9:00 pm	Discussion
9:00 pm - 9:10 pm	Courtney Roberts (University of Minnesota, United States)

"First d0 Metal-Catalyzed Alkyl-Alkyl Cross Coupling Enabled by a Redox-Active Ligand"

9:10 pm - 9:15 pm Discussion

9:15 pm - 9:25 pm **Rachel Baker** (California Institute of Technology, United States)
"Electrochemical Domino Carboxylation"

9:25 pm - 9:30 pm Discussion

Tuesday

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Polymers and Materials**
Discussion Leader: **Derek Wasylenko** (NOVA Chemicals, Canada)

9:00 am - 9:30 am **Aaron Sattler** (ExxonMobil, United States)
"Alkane Dehydrogenation & H₂ Removal Reactors"

9:30 am - 9:45 am Discussion

9:45 am - 10:15 am **Parisa Mehrkhodavandi** (UBC, Canada)
"Exploration of Ligand Hemilability in Cationic Indium Complexes for Ring Opening Polymerization"

10:15 am - 10:30 am Discussion

10:30 am - 11:00 am Coffee Break

11:00 am - 11:30 am **Michael Reynolds** (Shell USA, Inc, United States)
"Applying Green Chemicals as Modifiers for Controlling Inorganic Scale and Implications for Homogeneous Catalyst Design"

11:30 am - 11:45 am Discussion

11:45 am - 12:15 pm **David Steelman** (Dow Chemical Company, United States)
"Heterogeneous Catalyst Development for Ring Opening Polymerization of Alkylene Oxides"

12:15 pm - 12:30 pm Discussion

12:30 pm - 1:30 pm Lunch

1:30 pm - 4:00 pm Free Time

4:00 pm - 6:00 pm **Poster Session**

6:00 pm - 7:00 pm Dinner

7:30 pm - 9:30 pm **Computational Chemistry**
Discussion Leader: **Laurent Maron** (INSA, Toulouse University, France)

7:30 pm - 8:00 pm **Sharon Hammes-Schiffer** (Yale University, United States)

	"Proton-Coupled Electron Transfer in Catalysis and Energy Conversion"
8:00 pm - 8:15 pm	Discussion
8:15 pm - 8:45 pm	Stuart Macgregor (Heriot-Watt University, United Kingdom) "Modelling s-Alkane Structure and Reactivity in the Solid State"
8:45 pm - 9:00 pm	Discussion
9:00 pm - 9:10 pm	Amy Kynman (University of California, Berkeley, United States) "Lanthanide Photocatalyst for C (sp ³) - Halide Bond Activation and Functionalization: Importance of Metal-Ligand Cooperativity"
9:10 pm - 9:15 pm	Discussion
9:15 pm - 9:25 pm	William Whitehurst (Princeton University, United States) "C-H Activation by Cobalt & Iron Metallacycles"
9:25 pm - 9:30 pm	Discussion
Wednesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Alternative Energy, Energy Conversion and Electrocatalysis Discussion Leader: Michael Pegis (Sila NanoTechnologies, United States)
9:00 am - 9:30 am	James Mayer (Yale University, United States) "Reactive Hydrogen on Silicon and Oxide Surfaces"
9:30 am - 9:45 am	Discussion
9:45 am - 10:15 am	Gwendolyn Bailey (University of Minnesota, United States) "New Approaches to CO ₂ Reduction Using Atomically Precise Copper Nanoclusters"
10:15 am - 10:30 am	Discussion
10:30 am - 11:00 am	Coffee Break
11:00 am - 11:30 am	Shannon Stahl (University of Wisconsin-Madison, United States) "Exploring the Boundaries Between Thermal and Electrochemical Catalysis"
11:30 am - 11:45 am	Discussion
11:45 am - 12:15 pm	Ba Tran (Pacific Northwest National Laboratory, United States) "Mechanism-Guided Isolation and Reactivity of Monomeric and Dimeric Copper Hydrides"
12:15 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time

4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	f-Block Chemistry Discussion Leader: James Blakemore (University of Kansas, United States)
7:30 pm - 8:00 pm	Suzanne Bart (Purdue University, United States) "Understanding New Actinide-Element Multiple Bond Formation"
8:00 pm - 8:15 pm	Discussion
8:15 pm - 8:45 pm	Andrew Gaunt (Los Alamos National Laboratory, United States) "Molecular Transuranium Synthetic Chemistry"
8:45 pm - 9:00 pm	Discussion
9:00 pm - 9:10 pm	Md Estak Ahmed (Michigan State University , United States) "Electrocatalytic Ammonia Oxidization by Earth - Abundant Metal Complexes"
9:10 pm - 9:15 pm	Discussion
9:15 pm - 9:25 pm	Megan Fieser (University of Southern California, United States) "Catalytic Methods for the Chemical Upcycling of Waste Poly (Vinyl Chloride)"
9:25 pm - 9:30 pm	Discussion
Thursday	
7:30 am - 8:30 am	Breakfast
8:30 am - 9:00 am	Business Meeting <i>Nominations for the Next Vice Chair(s); Complete the GRC Evaluation Forms; Discuss Future Dates and Venue; Election of the Next Vice Chair(s)</i>
9:00 am - 12:30 pm	First Row Metals Discussion Leader: Warren Piers (University of Calgary, Canada)
9:00 am - 9:30 am	Nicholas Ball (Pomona College, United States) "Unlocking Fluorine: Activation of Sulfur(VI) Fluorides for New Sulfur-Fluorine Exchange (SuFEx) Reactions"
9:30 am - 9:45 am	Discussion
9:45 am - 10:15 am	Karsten Meyer (Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany) "“Super-Oxidized” Iron Nitrido and “Super-Reduced” Iron Nitrosyl Complexes in Tris-Carbene Coordination Spheres: How Iron Really Feels About it"
10:15 am - 10:30 am	Discussion
10:30 am - 11:00 am	Coffee Break
11:00 am - 11:30 am	Marcus Drover (The University of Windsor, Canada)

	"Exterior Decorating: Lewis Acid Secondary Coordination Spheres for Cooperative Reactivity"
11:30 am - 11:45 am	Discussion
11:45 am - 12:15 pm	Michael Whittlesey (University of Bath, United Kingdom) "Reactivity and Mechanisms in Transition Metal-Zinc Heterobimetallic Chemistry"
12:15 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Keynote Session: Active Sites and Mechanistic Probes Related to Catalytic Alkene Polymerization Discussion Leader: Patrick Holland (Yale University, United States)
7:30 pm - 8:15 pm	Clark Landis (University of Wisconsin-Madison, United States) "Empirical Determination of Reaction Mechanisms: Novel Instrumentation and Kinetic Modeling"
8:15 pm - 8:30 pm	Discussion
8:30 pm - 8:45 pm	General Discussion
8:45 pm - 9:00 pm	Closing Remarks
9:00 pm - 9:10 pm	Emily Tsui (University of Notre Dame, United States) "Sulfur Effects on Zinc Nucleophilicity"
9:10 pm - 9:15 pm	Discussion
9:15 pm - 9:25 pm	Deven Estes (University of Stuttgart, Germany) "Proton-Electron Transfers from Transition-Metal Hydrides to Bulk Metal Oxide Surfaces"
9:25 pm - 9:30 pm	Discussion
Friday	
7:30 am - 8:30 am	Breakfast
9:00 am	Departure

Contributors



**Gordon Research
Conferences**
Frontiers of Science





This material is based upon work supported by the U.S. Department of Energy, Office of Science, under Award Number DE-SC0023644. This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Inorganic Reaction Mechanisms (GRS)

Gordon Research Seminar

Mechanistic Studies and Operando Techniques to Innovate in Catalysis and Inorganic Chemistry

March 4 - 5, 2023

Chairs Lucie Nurdin and Michael Pegis

Grand Galvez

2024 Seawall Boulevard

Galveston, Texas, United States

Conference Program

Saturday

1:00 pm - 5:00 pm	Arrival and Check-in
3:30 pm - 3:45 pm	Introductory Comments by GRC Staff / Welcome and Introduction from the Chairs
3:45 pm - 4:30 pm	Keynote Session: Mechanisms of Electrochemical Energy Conversion Discussion Leader: Derek Wasylenko (NOVA Chemicals, Canada)
3:45 pm - 4:15 pm	James Mayer (Yale University, United States) "Thermodynamics and Kinetics of Hydrogen at Interfaces"
4:15 pm - 4:30 pm	Discussion
4:30 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Mechanisms of First Row Metals for Sustainable Catalysis Discussion Leader: Tianning Diao (New York University, United States)
7:30 pm - 7:50 pm	Jacklyn Hall (Argonne National Laboratory, United States) "Kinetic Evaluation of Reducible $\text{Li}_x\text{Mn}_2\text{O}_4$ -Supported Catalysts Synthesized by Oxidative Grafting"
7:50 pm - 8:00 pm	Discussion
8:00 pm - 8:20 pm	Jonathan Kephart (University of Washington, United States) "Capturing Surface Active Site Dynamics using Molecular Nanoclusters"
8:20 pm - 8:30 pm	Discussion
8:30 pm - 8:50 pm	Ross Koby (University of Minnesota, United States) "Ti-Catalyzed Alkyne Carboamination: More Fun Than a Barrel of Monkeys"
8:50 pm - 9:00 pm	Discussion
9:00 pm - 9:20 pm	Emma Cook (University of Virginia, United States) "Pendent Proton Relay Effects in Catalytic Dioxygen Reduction Mediated by Homogeneous Manganese Complexes"
9:20 pm - 9:30 pm	Discussion

Sunday

7:30 am - 8:30 am	Breakfast
9:00 am - 11:00 am	Inorganic Mechanisms Driven by Metal Ligand Cooperativity Discussion Leader: Carlos Rodriguez del Rio (Elsevier B.V., The Netherlands)
9:00 am - 9:20 am	Roel Bienenmann (Utrecht University, The Netherlands) "Mechanistic Investigation Into Copper(I) Hydride Catalyzed Formic Acid Dehydrogenation"
9:20 am - 9:30 am	Discussion
9:30 am - 9:50 am	Kaeden Teindl (University of British Columbia, Canada) "Role of Proton Transfer Driving Forces in CO ₂ Reduction Electrocatalysts with Tunable Secondary Coordination Spheres"
9:50 am - 10:00 am	Discussion
10:00 am - 10:20 am	Mengshan Ye (University of California, Berkeley, United States) "Reversible Alkyl-Group Migration between Iron and Sulfur in [Fe ₄ S ₄] Clusters"
10:20 am - 10:30 am	Discussion
10:30 am - 10:50 am	Amelia Reid (University of Virginia, United States) "Improving Co-Electrocatalytic Activity for CO ₂ Reduction through Redox Mediator Tuning and Catalyst Design"
10:50 am - 11:00 am	Discussion
11:00 am - 12:30 pm	Poster Session <i>Coffee will be served in the poster area from 11:00 am - 11:30 am</i>
12:30 pm - 1:30 pm	Lunch
1:30 pm - 2:30 pm	Mentorship Component: Career Panel Discussion Leader: Lucie Nurdin (Terraform Industries, United States)
1:30 pm - 2:30 pm	Panel Discussion <i>Careers in Academia, Industry, National laboratories and Science communication.</i> • James Mayer (Yale University, United States) • Carlos Rodriguez del Rio (Elsevier B.V., The Netherlands) • Renee Sifri (Merck, United States) • Ethan Crumlin (LBNL, United States) • Tianning Diao (New York University, United States) • Derek Wasylenko (NOVA Chemicals, Canada)
2:30 pm - 3:00 pm	Evaluation Period <i>Complete the GRS Evaluation Forms; Election of Future Chair(s)</i>
3:00 pm	Seminar Concludes

Contributors



This material is based upon work supported by the U.S. Department of Energy, Office of Science, under Award Number DE-SC0023644. This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.