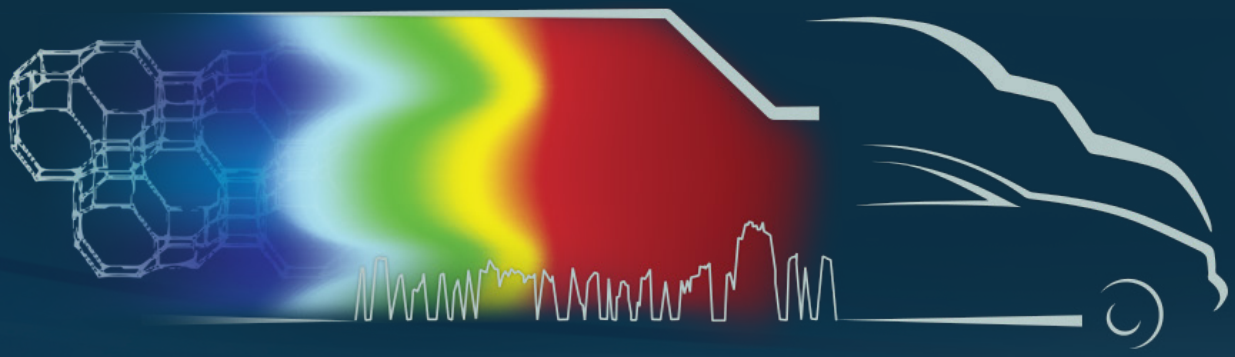
CLEERS



2020 CLEERS Virtual Workshop

September 14–18, 2020

Hosted and Coordinated by
Oak Ridge National Laboratory

Under the Guidance of
The DOE Advanced Engine Crosscut Team

https://cleers.org/event/2020-cleers-workshop

OVERVIEW

CLEERS Workshops are annual meetings open to all those who are interested in understanding and simulating the performance of exhaust emission control devices under realistic operating conditions. The Workshops provide an informal, focused forum to:

- Share recent experimental and computational simulation experience with advanced aftertreatment technologies;
- Enhance emissions control research collaborations among industry, universities, and DOE national laboratories; and
- Identify the most pressing pre-competitive research priorities for emissions control.

CLEERS Workshops feature invited presentations by internationally prominent researchers and a moderated discussion with an invited panel of industry experts.

Workshop participants are encouraged to contribute oral presentations and posters on the following (or related) technologies and topics.

TOPIC AREAS

Technologies:

- Passive NOx adsorbers (PNA)
- Hydrocarbon traps
- Selective catalytic reduction (SCR) of NOx by urea/ammonia
- Oxidation catalysts (DOC, MOC, etc.)
- Three-way catalysts (TWC)
- Diesel and gasoline particulate filters (DPF, GPF)
- Selective catalytic reduction of NOx by hydrocarbons (HC SCR)

Topics:

- Identification of reaction mechanisms (from micro-kinetic through global) and kinetic parameters
- Modeling strategies for improved accuracy and/or reduced computation time
- Drive cycle simulations of advanced vehicle/emissions control systems
- Formulation, evaluation, and simulation of catalysts with lower operating temperatures
- Multifunctional aftertreatment devices: catalyst coated filters, layered/zoned washcoats
- Integration of engines and emissions controls
- Durability
- Reductant (urea or fuel) delivery: spray modeling, decomposition processes, deposit formation

Find more information at https://cleers.org/event/2020-cleers-workshop

AGENDA

MONDAY, SEPTEMBER 14, 2020

11:00 a.m.	**WELCOME AND INTRODUCTION**	
11:05 a.m.	**Invited talk:** Single Atom Catalysts for Emission Control	Abhaya Datye (University of New Mexico)
11:55 a.m.	Pushing the Limits of Precious Metal Atom Economy for Three-Way-Catalysts (TWC): Thermally Stable and Highly Active Single Rh Atom Catalysts (Rh1/ceria)	Konstantin Khivantsev (Pacific Northwest National Lab)
12:20 p.m.	**Break**	
12:50 p.m.	Improving Platinum Group Metal Utilization for Emission Control Catalysts Through Thermally-Induced Restructuring of Core@Shell Nanoparticles	Alexander Hill (University of Michigan)
1:15 p.m.	Improved Ceria-Based Support With Enhanced Pt-CeO_2 Interaction Leading To Higher Activity and Stability for Catalytic Emission Control Reactions	Fudong Liu (University of Central Florida)
1:40 p.m.	Understanding of Low-Temperature Co Oxidation Active Sites on Atomically Dispersed Cu/CeO Synthesized via High-Temperature Synthesis	Yong Wang (Pacific Northwest National Laboratory)
2:05 p.m.	**Break**	
2:35 p.m.	**Panel Discussion:** Utilization of Platinum Group Metals in Emissions Control Catalysts	Saeed Alerasool (BASF) Wilfried Mueller (Umicore) Yong Wang (WSU/PNNL) Bill Epling (UVA)
4:15 p.m.	**END OF FIRST DAY SESSIONS**	

AGENDA

TUESDAY, SEPTEMBER 15, 2020

11:00 a.m.	**WELCOME AND INTRODUCTION**	
11:05 a.m.	**Invited talk:** GPF Modeling from Pore-Scale to the Entire Device	Petr Koci (Institute for Chemical Technology Prague)
11:55 a.m.	Gasoline Particulate Filter Technology for China6b with RDE	Mychal Taylor (NGK Insulators, Ltd.)
12:20 p.m.	**Break**	
12:50 p.m.	Improving GPF Filtration Performance Through Modeling Analysis	Xin Liu (Ford Motor Company)
1:15 p.m.	Towards Predictive Ash Accumulation and Transport Modeling	Grigorios Koltsakis (Aristotle University Thessaloniki)
1:40 p.m.	Hydration of Lubricant-Derived Ash in the Wall-Flow Particle Filter	Justin Kamp (Massachusetts Institute of Technology)
2:05 p.m.	**Break**	
2:35 p.m.	A Discrete DPF Filtration Model Considering Realistic Pore Size Distribution	Yujun Wang (Cummins)
3:00 p.m.	The Effect of NO_2/NOx Ratio on the Performance of a SCR Downstream of a SCR Catalyst on a DPF	Venkata Rajesh Chundru (Michigan Technological University)
3:25 p.m.	Mixed Metal Oxides for NO_2 Generation to Enhance SCRoF	Robert Henderson (Southwest Research Institute)
3:50 p.m.	A Modeling and Experimental Study on Deactivation of NO Oxidation Activity on Pt-Pd Catalyst with Hydrothermal Aging	Rama Krishna Dadi (Cummins)
4:15 p.m.	**END OF SECOND DAY SESSIONS**	

AGENDA

WEDNESDAY, SEPTEMBER 16, 2020

11:00 a.m.	**WELCOME AND INTRODUCTION**	
11:05 a.m.	**Invited talk:** System and Architecture Approach to Enable Diesel Engine Emission Reductions	Danan Dou, Eric Hruby (John Deere Power Systems)
11:55 a.m.	Transient Kinetic Analysis of the Reduction Half Cycle in the Standard SCR Redox Mechanism	Enrico Tronconi (Politecnico di Milano)
12:20 p.m.	**Break**	
12:50 p.m.	Using In Situ Electron Paramagnetic Resonance (EPR) Spectroscopy to Probe Reactivity and Relocation of Isolated Cu(II) Active Sites in Cu/SSZ-13 Selective Catalytic Reduction (SCR) Catalysts	Feng Gao (Pacific Northwest National Laboratory)
1:15 p.m.	Global Kinetic Models for Reduction and Oxidation Half-Cycles of The NH_3-SCR Redox Cycle: Application for Quantifying Active Cu Sites and Aging of Cu-zeolite Catalyst	Saurabh Joshi (Cummins Inc)
1:40 p.m.	Transient Tests to Assess the Cu Speciation in Cu-CHA Catalysts: Investigating Hydrothermal Aging Effects	Umberto Iacobone (Politecnico di Milano)
2:05 p.m.	**Break**	
2:35 p.m.	Development of Models for NH_3 SCR Storage and the Impacts of Hydrothermal Aging	Austin Ladshaw (Oak Ridge National Laboratory)
3:00 p.m.	Statistical Approach to Diesel Aftertreatment Accelerated Aging Performance Correlation to In-Use Population	Holmes Ahari (Fiat Chrysler Automobiles)
3:25 p.m.	Close-Coupled SCR: An Approach to Meet Ultra-Low NOx Requirements for Heavy-Duty Diesel Engines	John Kasab (AVL Powertrain Engineering Inc.)
3:50 p.m.	HCN Formation During NOx Removal by NH_3-SCR in the Exhaust of Natural Gas Engines	Deniz Zengel (Karlsruhe Institute of Technology)
4:15 p.m.	**END OF THIRD DAY SESSIONS**	

AGENDA

THURSDAY, SEPTEMBER 17, 2020

11:00 a.m.	**WELCOME AND INTRODUCTION**	
11:05 a.m.	**Stuart Daw Memorial Presentation:** Ammonia Control– The Next Frontier in Automotive Emissions Catalysis	Bean Getsoian (Ford Motor Company)
11:55 a.m.	Global Reaction Mechanism and Kinetic Parameters Identification for a Three-Way Catalyst Model in a System Simulation Context	Sana Loussaief (SIEMENS Digital Industries Software)
12:20 p.m.	**Break**	
12:50 p.m.	Three-Way Catalyst Reactivity of Novel High-Performance Fuels for SI/ACI Engine Emissions Control	Sreshtha Sinha Majumdar (Oak Ridge National Laboratory)
1:15 p.m.	Strategies for Overcoming Water Inhibition of Methane Oxidation Over Palladium-Based Catalysts	Patrick Lott (Karlsruhe Institute of Technology)
1:40 p.m.	A Novel Honeycomb for Both Downsizing and Significant PGM Saving	Mansour Masoudi (Emissol LLC)
2:05 p.m.	**Break**	
2:35 p.m.	**Poster Session #1**	
3:20 p.m.	**Break**	
3:30 p.m.	**Poster Session #2**	
4:15 p.m.	**END OF FOURTH DAY SESSIONS**	

AGENDA

FRIDAY, SEPTEMBER 18, 2020

11:00 A.M.	**WELCOME AND INTRODUCTION**	
11:05 a.m.	Flow and Forced Convection Heat and Mass Transfer Characteristics of Developed Laminar Flow in Channels of Relevance to Emissions Control Devices: Washcoated Monoliths and Asymmetric Particulate Filters	Tim Watling (Johnson Matthey)
11:30 a.m.	Effects of Hydrocarbon Structure on Adsorption Energetics on BEA Zeolite	Calvin Thomas (Oak Ridge National Laboratory)
11:55 a.m.	Condition-Dependent Pd Speciation and NO Adsorption in Pd/Zeolites	Chris Paolucci (University of Virginia)
12:20 p.m.	**Break**	
12:50 p.m.	Effect of Reduction and Re-oxidation on Pd Speciation in Pd-Zeolite Passive NOx Adsorbers	Robert Pace (University of Kentucky)
1:15 p.m.	Understanding the Cyclic Behavior of Passive NOx Adsorbers Under Low and High Concentrations of CO	Janos Szanyi (Pacific Northwest National Laboratory)
1:40 p.m.	Understanding the Degradation Mechanism of Pd/zeolite Based Passive NOx Adsorbers: The Interchange Between Particles and Cations	Kevin Gu (University of Virginia)
2:05 p.m.	**Break**	
2:35 p.m.	Improved NOx Storage Performance from Ethylene with Zeolite-Based Low Temperature NOx Adsorbers: Evidence of a Chemical Interaction	Joseph Theis (Ford Motor Company)
3:00 p.m.	Pd-dilution Approaches for More Sustainable Catalysts for Passive NOx Adsorption	Pranaw Kunal (Oak Ridge National Laboratory)
3:25 p.m.	Bimetallic PdCo/BEA Zeolites for Passive NOx Adsorption	Eleni Kyriakidou (University at Buffalo)
3:50 p.m.	Improving NOx Storage and CO Oxidation Abilities of Pd/SSZ-13 by Increasing its Hydrophobicity	Jaeha Lee (Seoul National University)
4:15 P.M.	**END OF FIFTH DAY SESSIONS**	

POSTER SESSIONS

THURSDAY, SEPTEMBER 17, 2020

***Poster Session #1: 2:35 p.m.; Poster Session #2: 3:30 p.m. (All Poster Rooms)**

Low Temperature Traps Poster Room	
Interconversion of Agglomerated Pd Domains and Ion-Exchanged Pd in CHA Zeolite Materials for Passive NOx Adsorption	Trevor Lardinois (Purdue University)
Influence of Pd Speciation on the Adsorption-Desorption Properties of Pd/BEA Hydrocarbon Traps for Diesel Emissions	Ryan Zelinsky (University of Virginia)
MOC & TWC Poster Room	
Cobalt as an Efficient Promoter in Low-loading Pd/BEA Catalysts for CH_4 Oxidation	Junjie Chen (University at Buffalo)
Effect of Lean/Rich Cycling on Catalytic Activity of a Methane Oxidation Catalyst	Natalia Diaz Montenegro (University of Virginia)
Structural changes of Rh/Al_2O_3 during CO oxidation	Silvia Marino (University of Virginia)
Effect of Slurry Processing on the Properties of Catalytically Active Aerogel Material	Ann Anderson (Union College)
TWC & DOC Poster Room	
Impact of Hydrothermal Aging on The Performance of Four Different Formulations of Prototype Three-Way Catalysts Under Exhaust Conditions Relevant to Propane Engines	Daekun Kim (University of Tennessee)
Low Temperature Oxidation of Novel High-Performance Fuels on Pt and Pd Catalysts	Fan Lin (Pacific Northwest National Laboratory)
Hydrothermally Stable Pd and Pt/CeO_2(core)@ZrO_2(shell) Catalysts for Low Temperature TWC Applications	Chih-Han Liu (University at Buffalo)
Non-Catalytic Gas-Phase NO Oxidation in the Presence of Decane	Chih-Han Liu (University at Buffalo)

POSTER SESSIONS

THURSDAY, SEPTEMBER 17, 2020

***Poster Session #1: 2:35 p.m.; Poster Session #2: 3:30 p.m. (All Poster Rooms)**

SCR Catalysts Poster Room	
Effects of Cu-Zeolite Topology on the Selective Catalytic Reduction of NOx with NH_3	Casey Jones (Purdue University)
Sulfur Poisoning and Hydrothermal Aging Effects on a Cu-SSZ-13 Selective Catalytic Reduction (SCR) Catalyst	Yu-Ren Chen (University of Virginia)
Kinetic Modeling of Sulfur Poisoning and Hydrothermal Aging Over Cu-SSZ-13 for NH_3-SCR	Lai Wei (University of Virginia)
SCR + SCO Poster Room	
Identification of the Role of Metal Oxide Component of Combined Metal Oxide-SSZ-13 Catalysts in Improving Low-Temperature Selective Catalytic Reduction of NOx by Ammonia	Tahrizi Andana (Pacific Northwest National Laboratory)
Fundamental Insights into the Active Sites and Kinetics of Ammonia Oxidation Over Cu/SSZ-13 Catalysts	Yiqing Wu (Pacific Northwest National Laboratory)
Passive Soot Oxidation Improvement in an SCR Coated DPF through Adding an Additional SCO Catalyst	Ben Jensen (Pacific Northwest National Laboratory)
SCR Systems Poster Room	
Alternative NH_3 Delivery Materials for Enabling Low-Temperature SCR	Zihao Zhang (Washington State University and Pacific Northwest National Laboratory)
Predictions of Urea Deposit Formation with CFD Using Autonomous Meshing and Detailed Urea Decomposition	Pengze Yang (Convergent Science Inc.)
A Modeling Study of an Advanced Ultra-Low NOx Aftertreatment System	Venkata Rajesh Chundru (Michigan Technological University)

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