

Tuesday, August 13, 2024

All times are EDT- Network: Marriott Bonvoy Conference - Password: **2Waterfront!**

08:00 – 09:00 AM **Welcome and Registration –**

08:00 – 09:00 AM **Breakfast Buffet**

Session Chair – Mehrdad Shahnam

09:00 – 09:20 AM **MFiX Development Updates**

Jeff Dietiker^{1,2}, ¹National Energy Technology Laboratory, Pittsburgh, PA, ²NETL Support Contractor, Pittsburgh, PA

09:20 – 09:40 AM **A Kinetic-based Model for Incompressible, Polydisperse, Fluid-particle Flows**

Chris Stafford¹, Rodney O. Fox¹, Alberto Passalacqua²; ¹Department of Chemical and Biological Engineering, Iowa State University, Ames, IA, ²Department of Mechanical Engineering, Iowa State University, Ames, IA

09:40 – 10:00 AM **Adaptation of the Vertical Upflow Phase Map of Wirth to Fluidized Dense Phase Conveying of Geldart A Powders and Validation of the Transition Boundaries by Eulerian Modelling with MFiX-TFM**

Prabu Balasubramanian, Andrew Cowell, Don McGlinchey, School of Computing, Engineering and Built Environment, Glasgow Caledonian University, United Kingdom

10:00 – 10:20 AM **On the Clustering and Settling Behavior of Polydisperse, Gas-solid Flows**

Sarah Beetham, Assistant Professor, Mechanical Engineering Oakland University, Rochester, MI

10:20 – 10:40 AM **A Filtered Coarse-grain CFD-DEM Approach for Simulating Fluidized Particles**

Sathvik Bhat¹, Yuan Yao², Pedram Pakseresh², Yi Fan², Jorg Theuerkauf³, Jesse Capecehatro¹, ¹Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI, ²Engineering and Process Science, Core R&D, The Dow Chemical Company, Lake Jackson, TX, ³Engineering and Process Science, Core R&D, the Dow Chemical Company, Midland, MI

10:40 – 10:50 AM Refreshment Break

Session Chair – Mary Ann Clarke

- 10:50 – 11:10 AM **Pioneering Real-Time In-Situ Machine Learning Integration for Multiphase Flow Analysis: A First-of-Its-Kind Workflow Demonstration with MFI-Exa**
*Aytekin Gel¹, Andrew Shao², Jordan Musser³, William Fullmer³;
¹ALPEMI Consulting, L.L.C., Tempe, AZ, ²Hewlett Packard Enterprise, ³National Energy Technology Laboratory, Morgantown, WV*
- 11:10 – 11:30 AM **Eulerian-Eulerian Two-Fluid Modeling of Non-spherical Particles Using DEM as a Closure Method to Determine the Deviation from the Kinetic Theory**
Ramon Lopez, Raymond Fontenot; CFD Research, 6820 Moquin Dr NW, Huntsville, Al
- 11:30 – 11:50 AM **Asynchronous GPU-Based DEM Solver Embedded in Commercial CFD Software with Polyhedral Mesh Support**
Alireza Kianimoqadam, Justin Lapp; University of Maine, Orono, ME
- 11:50 – 12:10 PM **Machine Learning of Transport Phenomena Simulated by Reduced-order Models Based on Proper Orthogonal Decomposition**
Paul Cizmas, Texas A&M University, College Station, TX

12:10 – 12:50 PM Luncheon Buffet

Session Chair – Janine Carney

- 12:50 – 1:10 PM **Graph Neural Networks for Unsteady Particle Drag Force Predictions**
Neil Ashwin Raj¹, Ze Cao², Danesh Tafti¹; ¹Dept. of Mechanical Engineering, Virginia Tech, Blacksburg, VA, ²School of Hydraulic Engineering, Dalian University of Technology, Dalian, China, ³Department of Computer Science, Stevens Institute of Technology, Hoboken, NJ
- 1:10 – 1:30 PM **Unraveling the Pyrolytic Behavior and Kinetics of Pure Polymers and Plastic-Rich Municipal Solid Waste Using Thermal Analysis**
Muhammad Aamir Bashir^{1,3}, Sittichai Natesakhawat^{1,3}, Mehrdad Shahnam², Ping Wang¹; ¹National Energy Technology Laboratory, Pittsburgh, PA, ²National Energy Technology Laboratory, Morgantown, WV, ³NETL Support Contractor, Pittsburgh, PA

- 1:30 – 1:50 PM **Phy-ChemNODE: A Physics-Enhanced Neural Ordinary Differential Equations Approach for Accelerating Stiff Chemical Kinetic Computations**
Pinaki Pal, Tadbhagya Kumar, Anuj Kumar, TRANSPORTATION AND POWER SYSTEMS DIVISION, ARGONNE NATIONAL LABORATORY
- 1:50 – 2:10 PM **Implementation of Detailed Polyethylene Pyrolysis Kinetics into CFD Simulations using Machine Learning**
Ross Houston¹, Hang Zhou^{1,2}; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV
- 2:10 – 2:30 PM **An Analytical Study on the Effect of Hydrodynamic and Electrostatic Forces on Particle Removal**
Abbas Khanmohammadi, Goodarz Ahmadi; Department of Mechanical and Aerospace Engineering, Clarkson University, Potsdam, NY
- 2:30 – 2:50 PM **Effectiveness Factor Estimates for General Catalyst Geometries**
John P. Wakefield¹, Jesse Capecehatro^{1,2}; ¹Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI, ²Department of Aerospace Engineering, University of Michigan, Ann Arbor, MI

2:50 – 3:00 PM Refreshment Break

Session Chair – Jordan Musser

- 3:00 – 3:20 PM **Predicting Biomass Comminution: Physical Experiment, Computational Particle-flow Simulation, Population Balance Model, and Deep Learning**
Yidong Xia, Physical Process Science & Realization Group, Idaho National Laboratory
- 3:20 – 3:40 PM **DEM Modeling of the Influence of Vibrational Forcing on the Flowability of Milled Biomass in Wedge-shaped Hoppers**
Nicholas Deak¹, Yimin Lu², Hariswaran Sitaraman¹, ¹National Renewable Energy Laboratory, Golden, CO, ²Texas Tech University, Lubbock, TX

3:40 – 4:00 PM

CFD-DEM Modeling of Fluidization Characteristics of Spherocylindrical Particles and Binary Mixtures

Ramesh Agarwal¹, Ling Zhou², Bo Wang², Ling Bai², ¹Department of Mechanical Engineering, Washington University in St. Louis, MO, ²Research Center of Fluid Machinery Engineering & Technology, Jiangsu University, Zhenjiang, China

4:00 – 4:20 PM

Computational Modeling of Wellbore Acoustics for Early-Kick Detection (EKD) using Logging-While-Drilling (LWD) Tools

Janine Carney¹, Felipe Maciel², Paulo Waltrich², Foad Haeri³; ¹National Energy Technology Laboratory, Albany, OR, ²Louisiana State University, Baton Rouge, LA, ³NETL Support Contractor, Pittsburgh, PA

4:20 – 4:40 PM

On the Essential Role of Nuclear Weapons Technologies in the Development of Particle Tracking Velocimetry for Flows of High Particle Concentrations

Franklin D. Shaffer; FDShaffer.net

4:40 PM

End of Day One

Wednesday, August 14, 2024

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08:00 – 09:00 AM Welcome and Registration –

08:00 – 09:00 AM Breakfast Buffet

Session Chair – William Fullmer

9:00 – 9:20 AM **MFIX-Exa Development Overview**
Jordan Musser, National Energy Technology Laboratory, Morgantown, WV

9:20 – 9:40 AM **Numerical Simulation of a Biogenic Fluid Catalytic Cracking (BFCC) Regenerator with MFIX-Exa**
Yupeng Xu^{1,2}, Jordan Musser¹, Mehrdad Shahnami¹; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV

9:40 – 10:00 AM **Effect of Instantaneous Local Solid Volume Fraction on Unsteady Drag Forces in Freely Evolving Particle Suspensions**
Ze Cao¹, Danesh. K. Tafti²; ¹School of Hydraulic Engineering, Dalian University of Technology, Dalian, China, ²Department of Mechanical Engineering, Virginia Tech, Blacksburg, VA

10:00 – 10:20 AM **CFP Regenerator Model Development**
Bruce D Adkins¹, Yupeng Xu^{2,3}, Mehrdad Shahnami², Jordan Musser²; ¹Oak Ridge National Lab, Oak Ridge, TN, ²National Energy Technology Laboratory, Morgantown, WV, ³NETL Support Contractor, Morgantown, WV

10:20 – 10:40 AM **ActivO: A Novel Active Machine Learning Framework for Rapid Simulation-driven Design Optimization**
Pinaki Pal, Transportation and Power Systems Division, Argonne National Laboratory

10:40 – 10:50 AM Refreshment Break

Session Chair – Ross Houston

10:50 – 11:10 AM **CFD Study of Airborne Transmission Using DRW Model in a Ventilated Office Room**
Amirmasoud Anvari, Goodarz Ahmadi; Department of Mechanical and Aerospace Engineering, Clarkson University, Potsdam, NY

Wednesday, August 14, 2024

- 11:10 – 11:30 AM **Enhancing Accuracy of Large Eddy Simulation for Particle-Laden Wall-Bounded Flows Through Stochastic Subgrid-Scale Fluctuations Modeling**
Farid Rousta¹, Goodarz Ahmadi¹, Bamdad Lessani²; ¹Department of Mechanical and Aerospace Engineering, Clarkson University, Potsdam, NY, ²Mechanical Engineering and Engineering Science, University of North Carolina at Charlotte, Charlotte, NC
- 11:30 – 11:50 AM **Computational Modeling of Proppants Transport in Rock Fractures**
Farid Rousta¹, Goodarz Ahmadi¹, Dustin Crandall²; ¹Department of Mechanical and Aerospace Engineering, Clarkson University, Potsdam, NY, ²National Energy Technology Laboratory
- 11:50 – 12:10 PM **Pore Morphology Method for Modeling Liquid Intrusion in Porous Media**
S. Gautam¹, Bhatta¹, A. Kumar¹, H.V. Tafreshi^{1,2}, B. Pourdeyhimi²; ¹Department of Mechanical and Aerospace Engineering, NC State University, Raleigh, NC, ²The Nonwovens Institute, NC State University, Raleigh, NC
- 12:10 – 12:30 PM **PMM-DPM Simulation of Aerosol Droplet Filtration Using a Coalescing Filter**
N. Bahatta¹, S. Gautam¹, A. Kumar¹, H.V. Tafreshi^{1,2}, B. Pourdeyhimi²; ¹Department of Mechanical and Aerospace Engineering, NC State University, Raleigh, NC, ²The Nonwovens Institute, NC State University, Raleigh, NC

12:30 – 1:10 PM Luncheon Buffet

Session Chair – David Huckaby

- 1:10 – 1:30 PM **Implementation of the Glued Sphere Discrete Element Method for Non-Spherical Particles in MFX Software**
Renjie Ke^{1,2}, Hang Zhou^{1,2}; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV
- 1:30 – 1:50 PM **Capturing O₂ Desorption Through Iso-conversional Kinetics for CFD Application**
Arthur Ndri Konan^{1,2}, Mary Ann Clarke¹; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV

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- 1:50 – 2:10 PM **Development of a Liquid Bridge Model for Particle Agglomeration and Defluidization in Plastic Pyrolysis**
Subhodeep Banerjee^{1,2}; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV
- 2:10 – 2:30 PM **Characterization of Solid Sorbent for Direct Air Capture of CO₂ using a CFD-based Methodology**
Hossain Aziz^{1,2}; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV
- 2:30 – 2:50 PM **Microwave Assisted Heating for Gasification**
RahulBabu Koneru^{1,2}, David Huckaby¹, Mehrdad Shahnam¹; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV
- 2:50 – 3:10 PM **Enhancing the Harris and Crighton PIC Stress Model with Bayesian Learning**
Akhil V. Marayikkottu^{1,2}; ¹National Energy Technology Laboratory, Morgantown, WV, ²NETL Support Contractor, Morgantown, WV
- 3:10 – 3:30 PM **Direct numerical simulation of flow past randomly distributed Platonic polyhedrons**
Aashish Goyal^{1,4}, Guodong Gai², Zihao Cheng³, Anthony Wachs^{1,2}; ¹Department of Chemical and Biological Engineering, University of British Columbia, Vancouver, Canada; ²Department of Mathematics, University of British Columbia, Vancouver, Canada; ³Department of Mechanical Engineering, University of British Columbia, Vancouver, Canada; ⁴National Energy Technology Laboratory, Morgantown, WV
- 3:30 PM Final Refreshment Break and the workshop concludes**

Thank you for supporting NETL’s 2024 Multiphase Flow Science Workshop! We appreciate all presenters and attendees!

Please send any feedback on this workshop including suggestions for future workshops to workshops@mfix.netl.doe.gov