**Tuesday, August 3, 2021**  
All times are Eastern Daylight Time

**Session Chair – William Rogers**

- **09:40 – 10:00 AM**  
  Log on, Webex Logistics  
  NETL Conference Services

- **10:00 – 10:20 AM**  
  Welcome and Introduction  
  Madhava Syamlal, NETL

- **10:20 – 11:00 AM**  
  Keynote Presentation: Multiscale Modeling & Simulations of Multiphase Flow at Unprecedented Resolution Using Machine Learning  
  S. Balachandar, University of Florida

- **11:00 – 11:20 AM**  
  A Convolutional Neural Network (CNN) based Drag Model for Particle-Fluid Two-Phase Flow  
  FeiFei Song, Tianjin University of Technology

- **11:20 – 11:40 AM**  
  Stochastic Modeling of Drag Forces in Euler-Lagrange Simulations of Particle-Laden Flows  
  Aaron Lattanzi¹, Vahid Tavanashad², Shankar Subramaniam², and Jesse Capecelatro¹, ¹University of Michigan, ²Iowa State University

- **11:40 – 12:00 PM**  
  Deep Learning Methods for Predicting Fluid Forces in Dense Ellipsoidal Particle Suspensions  
  Neil Ashwin Raj, Ze Cao, Nikhil Muralidhar, Danesh Tafti, Anuj Karpatne, Virginia Tech

- **12:00 – 12:20 PM**  
  A Machine Learning-based Interaction Model for Non-spherical Particles in Incompressible Flow  
  Soohwan Hwang, Jianhua Pan, Liang-Shih Fan, The Ohio State University

- **12:20 – 12:40 PM**  
  Physics Guided Neural Networks for Spherical Particle Drag Force Prediction in Assembly  
  Nikhil Muralidhar, Jie Bu, Ze Cao, Long He, Neil Ashwin Raj, Naren Ramakrishnan, Danesh Tafti, Anuj Karpatne, Virginia Tech

- **12:40 – 1:00 PM**  
  Break
Tuesday, August 3, 2021
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Session Chair – Mehrdad Shahnam

1:00 – 1:20 PM  CFD-Population Balance Modelling of Carbon Dioxide Dissolution for Geologic Sequestration
Alexander Vikhansky¹, Dmitry Eskin², Aditya Budaraju³, Yuri Leonenko⁴,
¹Siemens Digital Industries Software, ²The University of The West Indies,
³Siemens Digital Industries Software, ⁴University of Waterloo

1:20 – 1:40 PM  Numerical Simulation of Rock Fracture Coverage with Proppants during Hydraulic Fracturing
Farid Rousta,¹ Amir A. Mofakham,¹ Dustin Crandall,² Goodarz Ahmadi⁷,
¹Clarkson University, ²National Energy Technology Laboratory

1:40 – 2:00 PM  Numerical Simulation of Oil Well Cementing and Gas Migration Process
Amir A. Mofakham,¹ Farid Rousta,¹ Mehrdad Massoudi,² Eilis Rosenbaum,² Barbara Kutchko,² Goodarz Ahmadi⁵,¹ Clarkson University,
²National Energy Technology Laboratory

2:00 – 2:20 PM  Simulation-Based Digital Twins for Improved Asset Operation and Maintenance Management
Anchal Jatale, Ansys Inc.

2:20 – 2:40 PM  An Open-source One-dimensional Model for Bubbling Fluidized Bed Reactors
Gavin M. Wiggins¹ and Cornelius Emeka Agu²,¹Oak Ridge National Laboratory, ²Abbon AS

2:40 – 3:00 PM  Sensitivity Analysis of MFiX-PIC Parameters Using Nodenworks, PSUADE, and DAKOTA
Aytekin Gel, Justin Weber, Avinash Vaidheeswaran
National Energy Technology Laboratory

3:00 – 3:20 PM  Break
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Session Chair – Deepthi Chandramouli

3:20 – 3:40 PM  Multi-Fidelity Uncertainty Quantification for Gas-Solid Flows
Yuan Yao, Xun Huan, University of Michigan

3:40 – 4:00 PM  The “Gravity” of Combustion, Fluid and Soft Matter Research
John B. McQuillen¹, Daniel L. Dietrich¹, Suman Sinharay² ¹NASA Glenn Research Center, ²Universities Space Research Association

4:00 – 4:20 PM  Violent Fluidization and Erosion in Plume Surface Interactions
Matt Gorman, Juan Sebastian Rubio, Miguel X. Diaz-Lopez, Rui Ni
Johns Hopkins University

4:20 PM  Tuesday Session Ends
Wednesday, August 4, 2021
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9:40 – 10:00 AM   Log in

Session Chair – Mary Ann Clarke

10:00 – 10:20 AM  Heat and Mass Transfer in High-Temperature Particle–Gas Flows Under High-Flux Irradiation
Jingjing Chen¹, Apurv Kumar¹², Joe Coventry¹, Wojciech Lipinski¹, ¹The Australian National University, ²Federation University Australia

10:20 – 10:40 AM  CFD Modelling Biomass Gasification and Combustion with an Intra-particle Heterogenous Structure-Based Particle Model
Hao Luo¹, Xinyan Liu¹, Weigang Lin², Kim Dam-johanson², Hao Wu², ¹Wuhan University of Science and Technology, ²Technical University of Denmark

10:40 – 11:00 AM  Numerical Investigation into Biomass Gasification Using Fluidized Bed Gasifier
Hira Jaffer, M. Wasim Tahir
University of Engineering & Technology, Lahore, Pakistan

11:00 – 11:20 AM  A Method to Predict Fluidized Bed Particle Collision Speeds and Their Propensity to Agglomerate
Allan Runstedtler, Marc A. Duchesne
Natural Resources Canada/CanmetENERGY

11:20 – 11:40 AM  A New Multiphase CFD Erosion Model for Predicting Material Erosion from Sand Slurries
Amy B. McCleney, Southwest Research Institute

11:40 – 12:00 PM  Mixture Multiphase Model for Different Flow Regimes
Stephan Weller, Siemens Digital Industries Software

12:00 – 12:20 PM  Investigating Errors and Convergence in Stochastic Lagrangian-Eulerian Methods for Disperse Multiphase Flows
Jairo Vanegas, Noah Van Dam, University of Massachusetts Lowell

12:20 – 12:40 PM  On the Effect of Particle Froude Number in Sub-Grid Modeling of Gas-Solid Fluidized Flows
Christian C. Milioli, Fernando E. Milioli, University of Sao Paulo

12:40 – 1:00 PM    Break
2021 NETL Workshop on Multiphase Flow Science

Wednesday, August 4, 2021
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Session Chair – Avinash Vaidheeswaran

1:00 – 1:20 PM  Self-Disturbance Corrected Two-Way Coupled Euler-Lagrange Approach for Particle-Laden Flows with Heat Transfer on Arbitrary Shaped Grids
Sourabh V. Apte, Oregon State University

1:20 – 1:40 AM  Critical Sticking and Critical Slipping Convection Modes in Continuous Spatial Particle Atomic Layer Deposition
Julia Hartig, Davis C. Conklin, Alan W. Weimer, University of Colorado

1:40 – 2:00 PM  Computational Modeling of Structured Flow Phenomena in Vibrated Fluidized Beds
Qiang Guo, Yuxuan Zhang, Christopher M. Boyce, Columbia University

2:00 – 2:20 PM  An Easily Implementable General Self-induced Perturbation Correction Model for a Finite-sized Particle in Two-way Coupled Euler-Lagrange Simulations
Kai Liu\textsuperscript{1,2}, S. Balachandara\textsuperscript{1}, \textsuperscript{1}University of Florida, \textsuperscript{2}Zhejiang University

2:20 – 2:40 PM  Simulation and Modeling of Thermally Evolving, Moderately Dense Gas-Particle Flows
Sarah Beetham, Aaron Lattanzi, Jesse Capecelatro, University of Michigan

2:40 – 3:00 PM  Experimental Investigations of Settling Non-spherical Particles
Xu Xu, Jiacai Lu, Gretar Tryggvason, Rui Ni, Johns Hopkins University

3:00 – 3:20 PM  Break

Session Chair – Steven Rowan

Veeraraghava Raju Hasti, Purdue University

3:40 – 4:00 PM  Experimentally Measuring Contact Slipping and Rolling in Three-Dimensional Granular Spheres
Zackery A. Benson, Anton Peshkov, Nicole Y. Halpern, Derek C. Richardson, Wolfgang Losert, University of Maryland

4:00 – 4:20 PM  Fragmentation in Turbulence by Small Eddies
Yinghe Qi, Noah Corbitt, Carl Urbanik, Shiyong Tan, Ashwanth Salibindla, Rui Ni, Johns Hopkins University
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4:20 – 4:40 PM  Interactions between Liquid Interfaces and Shock-Laden Supersonic Flows: Near-Field Interfacial Physics
Prashant Khare, University of Cincinnati

4:40 – 5:00 PM  Simulation of the Transcritical Shock-Droplet Interaction
Bradley Boyd, Dorrin Jarrahbashi, Texas A&M University

5:00 PM  Wednesday Session Ends
2021 NETL Workshop on Multiphase Flow Science

Thursday, August 5, 2021
All times are Eastern Daylight Time

9:40 – 10:00 AM  Log in

Session Chair – Jeff Dietiker

10:00 – 10:20 AM  CFD-DEM Simulation and Experiment of Wet Particle Fluidization in Liquid-Injected Fluidized Beds
Leina Hua,¹ Qiushi Xu,¹ ² Raffaella Ocone,³ Ning Yang¹ ²
¹Chinese Academy of Sciences, ²University of Chinese Academy of Sciences, ³Heriot-Watt University

10:20 – 10:40 AM  The Structures of Pebbles Using the DEM Coupled with CFD for the Pebble Bed Reactors
Kyoung O. Lee, Benjamin S. Collins, Oak Ridge National Laboratory

10:40 – 11:00 AM  Flow patterns of capsule-shaped particle
Govind Sharma, Bahni Ray, Indian Institute of Technology, Delhi

11:00 – 11:20 AM  Numerical Modeling of Multiphase Cavitation Flow using Multiscale Bridging of Models at Different Scales
Jingsen Ma, Chao-Tsung Hsiao, Georges L. Chahine, Dynaflow, Inc.

Xianyang Chen, Jiacaï Lu, Gretar Tryggvason, Johns Hopkins University

11:40 – 12:00 PM  An Experimental and Computational Study of Supercritical Methane Injection Characteristics in CO2 Environment
Gihun Kim¹, Nelson Longmire², Ritesh Ghorpade¹, K. R. V. Manikantachari¹, Daniel Banuti², Subith Vasu¹,
¹ University of Central Florida, ²University of New Mexico

12:00 – 12:20 PM  Recent Advances in Positron Emission Particle Tracking for the Three-Dimensional Imaging of Industrial and Scientific Systems

12:20 – 12:40 PM  Quantifying the Effects of Transient Heating Conditions on Microchannel Flow Boiling Instabilities
Todd A. Kingston, Iowa State University

12:40 – 1:00 PM  Break
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Session Chair – Subhodeep Banerjee

1:00 – 1:20 PM  Cold Flow Investigations of a Plug Flow Reactor with Internal Recirculation for Pressurized Chemical Looping
Scott Champagne¹, Robin Hughes¹, Amanda Alain¹, Nicole Bond¹, Christopher McIntyre², Steven Montero¹, ¹Natural Resources Canada, CanmetENERGY, ²Hatch, Ltd.

1:20 – 1:40 AM  CPFD Analysis of a Commercial Scale Plug Flow Internal Recirculation Reactor for Use in Pressurized Chemical Looping Combustion
C. J. McIntyre¹, A. Kokourine¹, N. Bond², S. Champagne² R.W. Hughes²
¹Hatch, Ltd., ²Natural Resources Canada, CanmetENERGY

1:40 – 2:00 PM  A Numerical Study on Regenerator in the Fluid Catalytic Cracking Process
Babak Kashir¹, Raj Venuturumilli², Samir Khanna², Alberto Passalacqua¹, Rodney O Fox¹, ¹Iowa State University, ²BP, Naperville, IL

2:00 – 2:20 PM  Modeling Nuclear Fuels Coaters Using a Coupled ML–CFD Approach
Zachary Mills, Miroslav Stoyanov, Eddie Lopez Honorato, Charles Finney, John Hunn, Oak Ridge National Laboratory

2:20 – 2:40 PM  An Open-Source Library for Multi-Step Reactions in Spherical and Cylindrical Particles
John Wakefield¹, Aaron Lattanzi¹, Brennan Pech², Peter Ciesielski², Jesse Capecelatro¹, ¹University of Michigan, ²National Renewable Energy Laboratory

2:40 – 3:00 PM  CFD Simulation of Electrostatic Charging in Gas-Solid Fluidized Beds
Fahad Chowdhury¹, Manjil Ray², Alberto Passalacqua², Andrew Sowinski¹, Poupak Mehrani¹, ¹University of Ottawa, ²Iowa State University

3:00 – 3:20 PM  Break
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Session Chair – Yupeng Xu

3:20 – 3:40 PM  
Virus Transmission: How Airborne is “Airborne”?  
V. Kotteda¹, A. Badhan², V. Kumar²,³, C. Harris³, H. Janssen⁴  
¹University of Wyoming, ²University of Texas at El Paso, ³DeepVein Inc, ⁴Texas Tech University

3:40 – 4:00 PM  
Simulating the Formation of Granular Jets  
Sofiane Benyahia, National Energy Technology Laboratory

4:00 – 4:20 PM  
Accurate Drag, Lift, and Torque Correlations for the Family of Prolate Spheroids up to High Reynolds Numbers  
Sathish K. P. Sanjeevi¹, Jean F. Dietiker¹, Johan T. Padding², ¹National Energy Technology Laboratory, ²Delft University of Technology

4:20 – 4:40 PM  
Calibration of A Particle-In-Cell Simulation Model for Gravitational Settling Bed Application  
Aytekin Gel, Avinash Vaidheeswaran, Mary Ann Clarke, National Energy Technology Laboratory

4:40 PM  
Meeting Ends

Many thanks to all who presented and attended for your support of the NETL Workshop!

Feel free to send your feedback on this meeting and suggestions for future workshops to workshops@mfix.netl.doe.gov