2021 NETL Workshop on Multiphase Flow Science

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 Lattanzi[1], Vahid Tavanashad[2], Shankar Subramaniam[2], and Jesse Capecelatro[1], [1]University of Michigan, [2]Iowa 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

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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 Vikhansky [1], Dmitry Eskin[2], Aditya Budaraju [3], Yuri Leonenko[4],
[1]Siemens Digital Industries Software, [2]The University of The West Indies, [3]Siemens Digital Industries Software, [4]University 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 Ahmadi[1],
[1] Clarkson University, [2] National 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 Ahmadi[1],[1] Clarkson University, [2] National 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. Wiggins[1] and Cornelius Emeka Agu[2], [1]Oak Ridge National Laboratory, [2]Abbon AS

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

3:00 – 3:20 PM Break

2021 NETL Workshop on Multiphase Flow Science

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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. McQuillen[1], Daniel L. Dietrich[1], Suman Sinharay[2,] [1]NASA Glenn Research Center, [2]Universities 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

2021 NETL Workshop on Multiphase Flow Science

Wednesday, August 4, 2021
All times are Eastern Daylight Time

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 Chen[1], Apurv Kumar[1,2], Joe Coventry[1], Wojciech Lipinski[1], [1]The Australian National University, [2]Federation University Australia

10:20 – 10:40 AM **CFD Modelling Biomass Gasification and Combustion with an Intra-particle Heterogenous Structure-Based Particle Model**
Hao Luo[1], Xinyan Liu[1], Weigang Lin[2], Kim Dam-johanson[2], Hao Wu[2],*
[1] Wuhan University of Science and Technology, [2] Technical 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
All times are Eastern Daylight Time

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[1,2], S. Balachandara[1], [1]University of Florida, [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

3:20 – 3:40 PM **Denoising and Fuel Spray Droplet Detection from Light-Scattered Images Using Deep Learning**
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

Wednesday, August 4, 2021
All times are Eastern Daylight Time

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 Yang[1,2]
[1]Chinese Academy of Sciences, [2]University of Chinese Academy of Sciences, [3]Heriot-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.

11:20 – 11:40 AM **Interface Retaining Coarsening for Gas-Liquid Multiphase Flows**
Xianyang Chen, Jiacai 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 Kim[1], Nelson Longmire[2], Ritesh Ghorpade[1], K. R. V. Manikantachari[1], Daniel Banuti[2], Subith Vasu[1],
[1] University of Central Florida, [2]University 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**
C.R.K. Windows-Yule, J.P.K. Seville, A.L. Nicuşan. D. Werner and M.T. Herald, The University of Birmingham, UK

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

2021 NETL Workshop on Multiphase Flow Science

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

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 Champagne[1], Robin Hughes[1], Amanda Alain[1], Nicole Bond[1], Christopher McIntyre[2], Steven Montero[1], [1]Natural Resources Canada, CanmetENERGY, [2]Hatch, 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. McIntyre[1], A. Kokourine[1], N. Bond[2], S. Champagne[2] R.W. Hughes[2]
[1]Hatch, Ltd., [2]Natural Resources Canada, CanmetENERGY

1:40 – 2:00 PM **A Numerical Study on Regenerator in the Fluid Catalytic Cracking Process**
Babak Kashir[1], Raj Venuturumilli[2], Samir Khanna[2], Alberto Passalacqua[1], Rodney O Fox[1], [1]Iowa State University, [2]BP, 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 Wakefield[1], Aaron Lattanzi[1], Brennan Pech[2], Peter Ciesielski[2], Jesse Capecelatro[1], [1]University of Michigan, [2]National Renewable Energy Laboratory

2:40 – 3:00 PM **CFD Simulation of Electrostatic Charging in Gas-Solid Fluidized Beds**
Fahad Chowdhury[1], Manjil Ray[2], Alberto Passalacqua[2], Andrew Sowinski[1], Poupak Mehrani[1], [1]University of Ottawa, [2]Iowa State University

3:00 – 3:20 PM Break

2021 NETL Workshop on Multiphase Flow Science

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Session Chair – Yupeng Xu

3:20 – 3:40 PM **Virus Transmission: How Airborne is "Airborne"?**
V. Kotteda[1], A. Badhan[2], V. Kumar [2,3], C. Harris[3], H. Janssen[4]
[1]University of Wyoming, [2]University of Texas at El Paso, [3]DeepVein Inc, [4]Texas 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. Sanjeevi[1], Jean F. Dietiker[1], Johan T. Padding[2], [1]National Energy Technology Laboratory, [2]Delft 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