

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](#)

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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 Ahmadi¹,
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 Ellis Rosenbaum,² Barbara Kutchko,² Goodarz Ahmadi¹,
¹Clarkson University, ²National Energy Technology Laboratory
- 2:00 – 2:20 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
- 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 **Simulation-Based Digital Twins for Improved Asset Operation and Maintenance Management**
Anchal Jatale, Ansys Inc.
- 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, Jesse Capecelatro, 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 – 4:40 PM **ACCESS: Autonomous Characterisation and Calibration using
Evolutionary Simulation Software**
Andrei Leonard Nicusan, University of Birmingham, UK
- 4:40 PM **Tuesday Session Ends**

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 Chen¹, Apurv Kumar^{1,2}, 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 Luo^{1}, 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](#)

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. Balachandara¹, ¹University of Florida, ²Zhejiang University
- 2:20 – 2:40 PM **Simulation and Modeling of Thermally Evolving, Moderately Dense Gas-Particle Flows**
Sarah Beetham, Aaron Lattanzi, Jesse Capecehatro, University of Michigan
- 2:40 – 3:00 PM **Experimental Investigations of Settling Non-spherical Particles**
Xu Xu, Jiakai Lu, Gretar Tryggvason, Rui Ni, Johns Hopkins University
- 3:00 – 3:20 PM **Break**

Session Chair – Steven Rowan

- 3:20 – 3:40 PM **Denosing 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

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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](#)

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}
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 Cavitation and Two-phase Flow using a Multiscale Approach**
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, Jiakai 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 Banut², 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**
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](#)

Thursday, August 5, 2021

All times are Eastern Daylight Time

Session Chair – Subhodeep Banerjee

- 1:00 – 1:20 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
- 1:20 – 1:40 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.
- 1:40 – 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 Capecehatro¹, 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 Ray^{2}, Alberto Passalacqua², Andrew Sowinski¹, Poupak Mehrani¹*, ¹University of Ottawa, ²Iowa State University, *speaker
- 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. Kumar^{2,3}, 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 **Sensitivity Analysis of MFIX-PIC Parameters Using Nodeworks, PSUADE, and DAKOTA**
Aytekin Gel, Justin Weber, Avinash Vaidheeswaran, National Energy Technology Laboratory
- 4:40 PM Meeting Ends

Many thanks to all who present and attend 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

Event: **2021 NETL Workshop on Multiphase Flow Science Day 1**

Event address for attendees: <https://doe.webex.com/doe/onstage/g.php?MTID=e32aee9d41a0e28cb3ef8c6ee13103094>

Date and time: Tuesday, August 3, 2021 9:30 am Eastern Daylight Time (New York, GMT-04:00)

Duration: 7 hours

Event number: 199 654 7963

Event password: 0101

Audio conference: To receive a call back, provide your phone number when you join the event, or call the number below and enter the access code.

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Access code: 199 654 7963

Event: **2021 NETL Workshop on Multiphase Flow Science Day 2**

Event address for attendees: <https://doe.webex.com/doe/onstage/g.php?MTID=e4c0c5980154beb9d83317ff1a76c6ec8>

Date and time: Wednesday, August 4, 2021 9:30 am Eastern Daylight Time (New York, GMT-04:00)

Duration: 7 hours

Event number: 199 848 2220

Event password: 0101

Audio conference: To receive a call back, provide your phone number when you join the event, or call the number below and enter the access code.

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Access code: 199 848 2220

Event:

2021 NETL Workshop on Multiphase Flow Science Day 3

Event address for attendees:

<https://doe.webex.com/doe/onstage/g.php?MTID=e7b02c75b0abbe28cc298fce5e37386df>

Date and time:

Thursday, August 5, 2021 9:30 am Eastern Daylight Time (New York, GMT-04:00)

Duration:

7 hours

Event number:

199 442 6908

Event password:

0101

Audio conference:

To receive a call back, provide your phone number when you join the event, or call the number below and enter the access code.

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Access code: 199 442 6908