Tuesday, August 8, 2017 – Morgantown Marriott at Waterfront Place

7:00 – 8:00 AM
Registration
Continental Breakfast

8:00 – 8:05 AM
Welcome and Introduction
William Rogers, Multiphase Flow Science Team
National Energy Technology Laboratory

8:05 – 8:20 AM
NETL Multiphase Flow Research Overview
Madhava Syamlal, Senior Fellow Computational Engineering
National Energy Technology Laboratory

Session Chair – William Rogers

8:20 – 9:00 AM
Keynote Presentation: Virtual Process Engineering in Coarse-Grained Discrete Particle Methods
Wei Ge
State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences

9:00 – 9:20 AM
Macroscopic Modeling of the Flow of Dilute Emulsions in the Presence of Micro-Inertia
Antony N. Beris, Paul M. Mwasame and Norman J. Wagner, University of Delaware

9:20 – 9:40 AM
An Euler-Lagrange Ewald Summation Method for Simulating Electrically Charged Particle-Laden Flows
Jesse Capecelatro, Yuan Yao, University of Michigan

9:40 – 10:10 AM
Break

Session Chair – Tingwen Li

10:10 – 10:30 AM
Computational Study on Biomass Fast Pyrolysis Oil Yield: Developing a Predictive Model Which Includes Hydrodynamics of the Bubbling-to-Slugging Transition in a Laboratory-Scale Fluidized Bed
Emilio Ramirez\textsuperscript{1,2}, Tingwen Li\textsuperscript{3}, Mehrdad Shahnam\textsuperscript{3}, Stuart Daw\textsuperscript{1}, Charles Finney\textsuperscript{1}, \textsuperscript{1}Oak Ridge National Laboratory, \textsuperscript{2}University of Tennessee, \textsuperscript{3}National Energy Technology Laboratory

10:30 – 10:50 AM
CFD-DEM Modeling of the Formation of Producer Gas Contaminants During Biomass Gasification
Oluwafemi Oyedjei, Nourredine Abdoulmoumine, University of Tennessee

10:50 – 11:10 AM
Simulating Biomass Fast Pyrolysis Reactors by Combining High and Low-order Computational Models
Jessica Torres, Gavin Wiggins, and Charles Finney, Oak Ridge National Laboratory
11:10 – 11:30 AM  Application of an Efficient Discrete Particle model to Simulate an Industrial FCC Regenerator
Liqiang Lu, Sofiane Benyahia, National Energy Technology Laboratory

Ross Houston, Oluwafemi Oyedeji, Nourredine Abdoulmoumine, University of Tennessee

Paul Cizmas, Texas A&M University

12:10 – 1:10 PM  Lunch

1:10 – 1:20 PM  Reconvene and Afternoon Introduction

Session Chair – Mehrdad Shahnam

1:20 – 1:40 PM  Statistical Analysis on Large-Scale Direct Numerical Simulation of Gas-Solid Flow
Limin Wang, Wei Ge, Jinghai Li
Institute of Process Engineering, Chinese Academy of Sciences

1:40 – 2:00 PM  Macro-Scale Effects Over Meso-Scale Filtered Parameters in Gas-Solid Riser Flows
Christian C. Milioli, Joseph Mouallem, Norman Chavez-Cussy, Seyed R. A. Niaki, Fernando E. Milioli, University of São Paulo

2:00 – 2:20 PM  Validation and Uncertainty Quantification of MFIX-DEM Simulations of Horizontal Air Jets in a Semicircular Fluidized Bed of Geldart Group D Particles
Peiyuan Liu¹, William D. Fullmer¹,², Casey Q. LaMarche¹, Allan Issangya², Ray Cocco², and Christine M. Hrenya¹, ¹University of Colorado Boulder, ²Particulate Solid Research, Inc.

A. Bakshi¹,², Mehrdad Shahnam², T. Li², C. Altantzis¹,², A. Gel³, W. Rogers², A.F. Ghoniem¹, ¹Massachusetts Institute of Technology, ²National Energy Technology Laboratory, ³ALPEMI Consulting, LLC
2:40 – 3:00 PM  Sensitivity Analysis of Hopper Bin Discharge Simulations with Discrete Element Method  
Aytekin Gel¹,², Avinash Vaidheeswaran², Jordan Musser², Charles Tong³,  
¹ALPEMI Consulting, LLC, ²National Energy Technology Laboratory,  
³Lawrence Livermore National Laboratory

3:00 – 3:20 PM  Improved Partial Coupling for Multi-Phase Flow Solvers  
Husam A. Elghannay, Danesh K. Tafti, Virginia Polytechnic Institute and State University

3:20 – 3:50 PM  Break

Session Chair – Avinash Vaidheeswaran

3:50 – 4:10 PM  On Modeling Unsaturated Flow of a Liquid Through Multiple Layers of Thin, Swelling Porous Media  
A. Kaffel, K. Pillai, University of Wisconsin Milwaukee WI, USA

4:10 – 4:30 PM  Predicting Transmissivity of a Fracture Under Shearing  
Amir A. Mofakham¹, Mathew Stadelman²,³,²,∗, Goodarz Ahmadi¹,²,³, Kevin T. Shanley²,³,⁴, Dustin Crandall², ¹Clarkson University, ²National Energy Technology Laboratory, ³Oak Ridge Institute for Science Education, ⁴State University of New York at New Paltz, *Now affiliated with The MITRE Corporation

4:30 – 4:50 PM  Attrition Prediction Model for Chemical Looping and Other CFB Systems  
Nathan Galinsky, Samuel Bayham, Ronald Breault, National Energy Technology Laboratory

4:50 – 5:10 PM  A Discrete Particle Model for Simulating Carbon Capture with Encapsulated Carbonate Solutions  
Justin R. Finn, Janine E. Galvin, National Energy Technology Laboratory
Wednesday, August 9, 2017 – Morgantown Marriott at Waterfront Place

7:00 – 8:00 AM  Continental Breakfast
8:00 – 8:10 AM  Reconvene and Introduction

Session Chair – William Rogers

8:10 – 8:30 AM  Introducing New Experimental Facilities to Study Lagrangian Interfacial Dynamics of Turbulent Multiphase Flow
Rui Ni, Ashik Ullah Mohammad Masuk, Ashwanth Salibindla, The Pennsylvania State University

8:30 – 8:50 AM  Dynamic Structures in Bubbling Gas-Solid Fluidised Beds. The Effect of Local Granular Rheology
Victor Francia, Kaiqiao Wu, and Marc-Olivier Coppens, University College London

8:50 – 9:10 AM  Determination of Flow Patterns by Image Analysis of a Rectangular Spouted Bed
Jingsi Yang, Steven L. Rowan, Ronald W. Breault, Justin M. Weber, National Energy Technology Laboratory

9:10 – 9:30 AM  Ongoing Validation Efforts in Gas-Liquid Flows with Phase Change in System and CFD Codes
Caleb S. Brooks, University of Illinois at Urbana-Champaign

Qussai Marashdeh¹, Fernando Teixeira², ¹Tech4Imaging LLC, ²The Ohio State University

9:50 – 10:20 AM  Break

Session Chair – William Fullmer

10:20 – 10:40 AM  Influence of the Wall Boundary Conditions and Particle Interactions on an Annular Fluidized Bed Reactor
Mohammed N. Khan, Tariq Shamim, Masdar Institute of Science and Technology

10:40 – 11:00 AM  Modification of the Modal Characteristics of a Square Cylinder Wake Obstructed by a Multi-Scale Array of Obstacles
Jonathan Higham, University of Sheffield
2017 NETL Workshop on Multiphase Flow Science

11:00 – 11:20 AM Experimental Study and CFD Simulation of a Down-Flow Bubble Column
Mutharasu L.C.1, Mayur Sathe1, Dinesh V. Kalaga2, Derek Griffin3, Krishnaswamy Nandakumar1, J.B. Joshi4, 1Louisiana State University, 2City College of New York, 3LanzaTech, 4Homi Bhabha National Institute, Mumbai, India.

11:20 – 11:40 AM Simulation of Particulate Flows Using a Hybridized Particle-in-Cell and Direct Simulation Monte Carlo Method
Aaron Morris, Purdue University

11:40 – 12:00 PM Linear Solver Performance Analysis of MFIX Integrated with a Next Generation Computational Framework
VMK Kotteda1, V Kumar1, W Spotz2, A Rodriguez1, A Schiaffino1, A Chattopadhyay1, 1University of Texas at El Paso, 2Sandia National Laboratories

12:00 – 1:00 PM Lunch

Session Chair – Arthur Konan

1:00 – 1:10 PM Reconvene and Afternoon Introduction

1:10 – 1:30 PM Improved Speed and Reliability of Averaged Multiphase Flow Calculations for Use in Combined 1D-CFD Multiphase Flow Process Simulations: Experimental Validation Against PipeFractionalFlow and Multiphase CFD Codes
Anand Nagoo, University of Texas

1:30 – 1:50 PM A DEM Study of Spontaneous Granular Structure Formation in a Cylindrical Vessel Under Orbital Motion
Jielin Yu1, Chunliang Wu2, Oladapo Ayeni3, Krishnaswamy Nandakumar1, J. B. Joshi1, Mayank Tyagi1, Shankar Ghosh3, 1Louisiana State University, 2SABIC, 3Tata Institute of Fundamental Research, India

1:50 – 2:10 PM Heat Transfer in Assemblies of Spherical and Ellipsoidal Particles
Long He, Danesh Tafti, Virginia Polytechnic Institute and State University

2:10 – 2:30 PM Data-Driven Smart CFD Proxy: Applications of Big Data Analytics & Machine Learning in Computational Fluid Dynamics
Shahab D. Mohaghegh1, Amir Ansari1, Mehrdad Shahnam2, Jean-Francois Dietiker2, Ebrahim Fathi1, Ali Takbiri1, 1West Virginia University, 2National Energy Technology Laboratory
2:30 – 2:50 PM  Simplified Soft-Sphere Collision Model for Fluid-Particle Systems  
Husam A. Elghannay, Danesh K. Tafti, Virginia Polytechnic Institute and State University

2:50 – 3:10 PM  Numerical Simulation and Experimental Study of a Small-Scale Circulating Fluidized Bed  
Yupeng Xu, Jordan Musser, Tingwen Li, Balaji Gopalan, Rupen Panday, Jonathan Tucker, Greggory Breault, William Rogers, National Energy Technology Laboratory

3:10 – 3:20 PM  Technical Meeting Wrap Up

Posters

MFIX into Matlab source code  
Ben Barrowes, Barrowes Consulting

Radial Flow Pulse Jet Mixing (RFPJM)  
John VanOsdol, National Energy Technology Laboratory
2017 NETL Workshop on Multiphase Flow Science

Thursday, August 10, 2017 – Morgantown Marriott at Waterfront Place

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<td>8:00 – 8:10 AM</td>
<td>Welcome to the NETL Multiphase Flow Science Session</td>
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<td>8:10 – 8:30 AM</td>
<td>MFiX Suite and Exascale Computing – Development Path</td>
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<td>Jordan Musser, National Energy Technology Laboratory</td>
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<td>8:30 – 8:45 AM</td>
<td>MFiX 17.1 Overview</td>
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<td>Jeff Dietiker, Justin Weber, National Energy Technology Laboratory</td>
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<td>8:45 – 10:30 AM</td>
<td>MFiX 17.1 Tutorials and Hands-on Assistance</td>
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<td>10:30 – 10:40 AM</td>
<td>Break</td>
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<td>10:40 – 12:00 PM</td>
<td>MFiX Optimization Toolset and Nodeworks</td>
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<td>Dirk Van Essendelft, Justin Weber, National Energy Technology Laboratory</td>
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