2017 NETL Workshop on Multiphase Flow Science

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[1,2], Tingwen Li[3], Mehrdad Shahnam[3], Stuart Daw[1], Charles Finney[1], [1]Oak Ridge National Laboratory, [2]University of Tennessee, [3]National Energy Technology Laboratory

10:30 – 10:50 AM **CFD-DEM Modeling of the Formation of Producer Gas Contaminants During Biomass Gasification**
Oluwafemi Oyedeji, 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

11:30 – 11:50 AM **Development of a Comprehensive Computational Fluid Dynamic and Discrete Element Model of Biomass Fast Pyrolysis in a Bubbling Fluidized Bed Reactor**
Ross Houston, Oluwafemi Oyedeji, Nourredine Abdoulmoumine, University of Tennessee

11:50 AM – 12:10 PM **A Method for Generating Reduced Kinetics Mechanisms used for Numerical Modeling of Reactive Flows**
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 Liu[1], William D. Fullmer[1,2], Casey Q. LaMarche[1], Allan Issangya[2], Ray Cocco[2], and Christine M. Hrenya[1], [1]University of Colorado Boulder, [2]Particulate Solid Research, Inc.

2:20 – 2:40 PM **CFD-DEM Simulations of Bubbling Fluidization: Identification of Critical Model and Numerical Parameters**
A. Bakshi [1,2], M. Shahnam[2], T. Li[2], C. Altantzis [1,2], A. Gel[3], W. Rogers[2], A.F. Ghoniem[1], [1]Massachusetts Institute of Technology, [2]National Energy Technology Laboratory, [3]ALPEMI Consulting, LLC

2:40 – 3:00 PM **Sensitivity Analysis of Hopper Bin Discharge Simulations with Discrete Element Method**
Aytekin Gel[1,2], Avinash Vaidheeswaran[2], Jordan Musser[2], Charles Tong[3], [1]ALPEMI Consulting, LLC, [2]National Energy Technology Laboratory, [3]Lawrence 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. Mofakham[1], Mathew Stadelman[2, 3, *], Goodarz Ahmadi[1, 2, 3], Kevin T. Shanley[2, 3, 4], Dustin Crandall[2]*, [1]Clarkson University, [2]National Energy Technology Laboratory, [3]Oak Ridge Institute for Science Education, [4]State 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

2017 NETL Workshop on Multiphase Flow Science

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

9:30 – 9:50 AM **A Multidimensional Approach to Multi-Phase Flow Instrumentation Using Capacitive Sensors**
Qussai Marashdeh[1], Fernando Teixeira[2], [1]Tech4Imaging LLC, [2]The 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

11:00 – 11:20 AM **Experimental Study and CFD Simulation of a Down-Flow Bubble Column**
Mutharasu L.C.[1], Mayur Sathe[1], Dinesh V. Kalaga[2], Derek Griffin[3], Krishnaswamy Nandakumar[1], J.B. Joshi[4], [1]Louisiana State University, [2]City College of New York, [3]LanzaTech, [4]Homi 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 Kotteda[1], V Kumar[1], W Spotz[2], A Rodriguez[1], A Schiaffino[1], A Chattopadhyay[1], [1]University of Texas at El Paso, [2]Sandia 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 Yu[1], Chunliang Wu[2], Oladapo Ayeni[1], Krishnaswamy Nandakumar[1], J. B. Joshi[1], Mayank Tyagi[1], Shankar Ghosh[3], [1]Louisiana State University, [2]SABIC, [3]Tata 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. Mohaghegh[1], Amir Ansari[1], Mehrdad Shahnam[2], Jean-Francois Dietiker[2], Ebrahim Fathi[1], Ali Takbiri[1], [1]West Virginia University, [2]National 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

7:00 – 8:00 AM	**Continental Breakfast**
8:00 – 8:10 AM	**Welcome to the NETL Multiphase Flow Science Session**
8:10 – 8:30 AM	**MFiX Suite and Exascale Computing – Development Path** *Jordan Musser*, National Energy Technology Laboratory
8:30 – 8:45 AM	**MFiX 17.1 Overview** *Jeff Dietiker, Justin Weber*, National Energy Technology Laboratory
8:45 – 10: 30 AM	**MFiX 17.1 Tutorials and Hands-on Assistance** *MFS Staff,* National Energy Technology Laboratory
10:30 – 10:40 AM	**Break**
10:40 – 12:00 PM	**MFiX Optimization Toolset and Nodeworks** *Dirk Van Essendelft, Justin Weber,* National Energy Technology Laboratory
12:00 – 1:00 PM	**Lunch**