

Tuesday, August 7, 2018 – University of Houston Student Center South – Theater

- 7:00 – 8:00 AM **Registration – Theater**
Continental Breakfast – Space City Room
- 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 – 8:40 AM **Opportunities and Challenges in Multiphase CFD Modeling in Upstream Oil and Gas**
Madhusuden Agrawal, BP America
- 8:40 – 9:00 AM **Exploiting Multiphase Slug Flow for Controlled Manufacturing of Uniform Crystals**
Mo Jiang, Virginia Commonwealth University
- 9:00 – 9:20 AM **Simulation of a Dual Circulating Fluidized Bed Reactor Combusting Coal by Chemical Looping with Oxygen Uncoupling**
Zachary Reinking, Kevin Whitty, JoAnn Lighty, University of Utah
- 9:20 – 9:40 PM **Reduced Chemical Mechanism for Chemical Looping with Oxygen Uncoupled Combustion System**
Hong-Shig Shim¹, Dave Wang¹, Kevin Davis¹, James Parker², Kevin Whitty³, ¹Reaction Engineering International, ²CPFD, ³University of Utah
- 9:40 – 10:00 AM **Break**

Session Chair – William Fullmer

- 10:00 – 10:20 AM **Direct Numerical Simulation of Low-Mach Reacting Gas-Solid Flows Using a Penalization Method**
B. Hardy, G. Winckelmans, J. De Wilde Université Catholique de Louvain
- 10:20 – 10:40 AM **Variation of Drag, Lift, and Torque in a Suspension of Ellipsoidal Particles**
Long He, Danesh Tafti, Virginia Tech
- 10:40 – 11:00 AM **Understanding Fluid-Particle Interaction in Structured Environments by Direct Numerical Simulation**
Chenguang Zhang, A'mer Shamleh, J. Joshi, Chunliang Wu, K. Nandakumar, Louisiana State University



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- 11:00 – 11:20 AM **3D Modelling of Non-Spherical Particulate Systems**
Vivek Srinivasan, Danesh Tafti, Virginia Tech
- 11:20 – 12:20 AM **Keynote Presentation: Pragmatic Approach for Modeling Industrial Scale Gas-Solids Reacting Flows**
Sreekanth Pannala, SABIC

12:20 – 1:20 PM Lunch - Ballroom

Session Chair – Mehrdad Shahnam

- 1:20 – 2:20 PM **Keynote Presentation: Multiscale Dynamics in Turbulent Bubbly Flows**
Rui Ni, Pennsylvania State University
- 2:20 – 2:40 PM **Dynamically Structured Fluidized Beds: Controlled Mixing Under Oscillatory Flows**
Victor Francia, Kaiqiao Wu, Marc-Olivier Coppens, University College London
- 2:40 – 3:00 PM **MRI of Bubble and Jet Injection into Fluidized Beds**
*Christopher M. Boyce^{1,2}, Alexander Penn^{1,3}, Maxim Lehnert¹, Klaas P. Pruessmann³, Christoph R. Müller¹,
¹ETH Zurich, ²Columbia University, ³University of Zurich and ETH Zurich*
- 3:00 – 3:20 PM **Triboelectric Charging and Electrostatic Effects in Granular and Particle-Laden Flows**
J. Kolehmainen, X. Liu, A. Ozel, S. Sundaresan, Princeton University
- 3:20 – 3:40 PM **Flow Field Characterization of Slug Flow Using PIV and CTA Techniques**
T. Kim, E. Pereyra, C. Sarica, University of Tulsa
- 3:40 – 4:00 PM Break



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Session Chair – Jeff Dietiker

- 4:00 – 4:20 PM **Preferential Concentration of Particles by Turbulence**
Amir Mofakham, Goodarz Ahmadi, Clarkson University
- 4:20 – 4:40 PM **Machine Learning Based Filtered Drag Force Model**
Yundi Jiang, Jari Kolehmainen, Yile Gu, Yannis Kevrekidis, Ali Ozel, Sankaran Sundaresan, Princeton University
- 4:40 – 5:00 PM **Data-driven Closure Framework for Multiphase Turbulence Modeling**
Sarah Beetham, Jesse Capecelatro, University of Michigan
- 5:00 – 5:20 PM **Effects of Sub-Grid Gas Turbulence over the Meso-Scale Hydrodynamics of Fluidized Gas-Solid Flows**
Christian Milioli, Joseph Mouallem, Seyed Niaki, Fernando Milioli, University of São Paulo
- 5:20 PM **Tuesday Session Ends**
- 5:30 PM **Reception – Space City Room**
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2018 NETL Workshop on Multiphase Flow Science



Wednesday, August 8, 2018 – University of Houston Student Center South - Theater

7:00 – 8:00 AM Continental Breakfast – Space City Room

8:00 AM Reconvene

Session Chair – Janine Carney

8:00 – 9:00 AM **Keynote Presentation: Improvements to Point-Particle Approach to Capture Fully-Resolved Physics and Development of Next Generation Euler-Lagrange Framework**
S. Balachandar, University of Florida

9:00 – 9:20 AM **Understanding and Modeling the Effect of Clusters on Heat Transfer in Gas-Solid Suspensions**
Jesse Capecehatro, University of Michigan

9:20 – 9:40 AM **Kinematic Waves from a Particle-resolved Simulation of a Fluidized-bed-like System**
G. Zhou¹, D. Willen¹, Y. Zhang¹, A. Prosperetti², ¹Johns Hopkins University, ²University of Houston

9:40 – 10:00 AM **Modified Kinetic Theory for the Flow of Dense Particulate Mixtures and Granular Materials**
Yifei Duan¹, Zhi-Gang Feng¹, Efstathios Michaelides², ¹University of Texas at San Antonio, ²Texas Christian University

10:00 – 10:20 AM Break

Panel Discussion Moderator: – S. Pannala, SABIC

10:20 – 12:00 PM **PANEL DISCUSSION: “How Can Multiphase Flow Modeling Have the Same Impact on Process Industry as Single-Phase Flow Modeling?”**
S. Pannala¹, James Parker², Madhava Syamlal³, Xiao-Hui Wu⁴, Krishnaswamy Nandakumar⁵, ¹SABIC, ²CPFD, ³National Energy Technology Laboratory, ⁴ExxonMobil, ⁵Louisiana State University

12:00 – 1:00 PM Lunch - Ballroom



2018 NETL Workshop on Multiphase Flow Science



Wednesday, August 8, 2018 – University of Houston Student Center South - Theater

Session Chair – Avinash Vaidheeswaran

- 1:00 PM **Reconvene**
- 1:00 – 1:20 PM **Multiscale Modeling of Liquid Spray from Stripping of Co-Current Liquid Film and Droplet Evaporation**
Prasad Kalghatgi, Christian Chauvet, Wood Automation and Control
- 1:20 – 1:40 PM **Numerical Simulation of Liquid Jet Disintegration, Spray Formation, and Combustion at High Pressures**
Dorriin Jarrahbashi, Texas A&M University
- 1:40 – 2:00 PM **Insights into Gas-Liquid Flow Systems Using Computational Fluid Dynamics Simulations of Various Petroleum Engineering Applications**
Mayank Tyagi, Louisiana State University
- 2:00 – 2:20 PM **Effect of Thermo-Physical Properties on Multiphase Flow Modeling**
Dale Erickson, Wood Automation & Control
- 2:20 – 2:40 PM **Advancement Measurement Techniques for Validation of Computational Fluid Dynamics (CFD)**
Multhanna Al-Dahhan, Missouri University of Science and Technology

2:40 – 3:00 PM **Break**

Session Chair – Justin Finn

- 3:00 – 3:20 PM **Cold Flow Analysis for a Scaled Bubbling Fluidized Bed with Various Fuel and Bed Material Types**
Ali Sivri, Amoolya Lalsare, Cosmin Dumitrescu, John Hu, West Virginia University
- 3:20 – 3:40 PM **CFD Simulation of Hydrodynamics of Ebullated Bed Reactor (EBR) for Heavy Oil Upgrading**
Saad Saleh¹, Shakir Ahmed², Mohammed Sanam¹, Salah Ali³, Harith Alani³, ¹University of Tikrit, ²Ministry of Oil, Iraq, ³Petroleum Research and Development Centre, Iraq
- 3:40 – 4:00 PM **Dakota Integrated with MFIX for UQ Analysis: Sensitivity of Particle Size on Pressure in Fluidized Bed DEM Simulations**
VMK Kottedda¹, Vinod Kumar¹, William Spitz², ¹University of Texas at El Paso, ²Sandia National Laboratories
- 4:00 PM **Technical Meeting End**



2018 NETL Workshop on Multiphase Flow Science



Thursday, August 9, 2018 – University of Houston Student Center South - Theater

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| 7:00 – 8:00 AM | Continental Breakfast – Space City Room |
| 8:00 – 8:10 AM | Welcome to the NETL Multiphase Flow Science Session
<i>William Rogers, National Energy Technology Laboratory</i> |
| 8:10 – 8:40 AM | MFiX and Exascale Computing – Development Update
<i>Jordan Musser, National Energy Technology Laboratory</i> |
| 8:40 – 9:40 AM | MFiX Suite Development Update
<i>Jeff Dietiker, National Energy Technology Laboratory</i> |
| 9:40 – 10:00 AM | Break |
| 10:00 – 10:45 AM | MFiX Suite Quality Assurance Program
<i>Avinash Vaidheeswaran, National Energy Technology Laboratory</i> |
| 10:45 – 11:45 PM | MFiX Optimization Toolset and Uncertainty Quantification Toolset
<i>Justin Weber, William Fullmer, Aytekin Gel, National Energy Technology Laboratory</i> |
| 12:00 – 1:00 PM | Lunch and End of Workshop – Box Lunches |

Posters

Discrete Particle Modeling of Carbon Capture Using Semipermeable Elastic Microcapsules

Justin Finn, Janine Galvin, National Energy Technology Laboratory

The Effect of Particle Size on Tribocharging

X. Lui, I. Nwogbaga, P. Saba, J. Kolehmainen, A. Ozel, S. Sundaresan, Princeton University

Particle Distribution and Deposition in a Rock Fracture

Amir Mofakham¹, G. Ahmadi^{1,2,3}, M. Stadelman³, K. Shanley^{2,3,4}, D. Crandall², ¹Clarkson University, ²National Energy Technology Laboratory, ³Oak Ridge Associated Universities, ⁴State University of New York

Bubbletree: A Rigorous Algorithm for Lagrangian Tracking and Statistical Analysis of Bubble or Cluster Motion and Flux within 3D Fluid Bed Simulations

Kyle Buchheit, NETL

Characterization of Hydrodynamics for Split Photobioreactor via Radioactive Particle Tracking (RPT) Technique

Laith Sabri, Abbas Sultan, Multhanna Al-Dahhan, Missouri University of Science and Technology

MFIX Integrated with Trilinos: First and Second Generation Preconditioned Linear Solvers Performance Analysis

Vinod Kumar, VMK Kotteda, William Spatz, A. Rodriguez, A. Schiaffino, University of Texas at El Paso

Advancing Hydrodynamics and Scale-up of Gas-Solid Systems via Sophisticated Measurement Techniques

Muthanna Al-Dahhan, Premkumar Kamalanathan, Haider Taofeeq, Neven Ali, A Efhaima, Missouri University of Science and Technology

Accelerating Computational Fluid Dynamics Using TensorFlow

Dirk VanEssendelft, Opeoluwa Owoyele, Kyle Buchheit, National Energy Technology Laboratory

Accuracy of DRW Stochastic Turbulence Models

Amir Mofakham, Goodarz Ahmadi, Clarkson University



2018 NETL Workshop on Multiphase Flow Science



Posters

An Investigation of Chemical Kinetics of Eastern Coal and Biomass Catalytic Gasification

Amoolya Lalsare, Yuxin Wang, Basel Rasheed, Ali Sivri, Cosmin Dumitrescu, Jianli Hu, West Virginia University

The Effect of Industrial Heat Exchanger Internals Structure on the Gas Holdup of Pilot Plant Bubble Column for Fischer Tropsch Synthesis

Multanna Al-Dahhan, Hayder Alnaseri, Joshua Schlegel, Missouri University of Science and Technology

Optimization and Uncertainty Quantification Toolsets

Justin Weber, William Fullmer, Aytekin Gel, National Energy Technology Laboratory