2019 NETL Workshop on Multiphase Flow Science

This year's workshop is dedicated to the memory of our multiphase flow research colleagues:
Dr. Charles Stuart Daw - March 16, 1950 - July 2, 2019
Dr. John Steven "Jack" Halow – September 1, 1942 – June 30, 2019

Tuesday, August 6, 2019 – Marriott at Waterfront Place – Salon E

7:00 – 8:00 AM Registration – Foyer F-H

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

8:05 – 8:20 AM **Commemoration of Dr. Daw and Dr. Halow**
Charles Finney
Oak Ridge National Laboratory

8:20 – 8:40 AM **NETL Multiphase Flow Research Overview**
Madhava Syamlal, Senior Fellow Computational Engineering
National Energy Technology Laboratory

Session 1: Chair – William Rogers

8:40 – 9:00 AM **Interactions of Particles with Flow Structures in Turbulent Channel Flows**
Amir Abdollahi Mofakham, Goodarz Ahmadi and John McLaughlin, Clarkson University

9:00 – 9:20 AM **Identifying Multiphase Turbulence Models Using Sparse Regression with Embedded Form Invariance**
Sarah Beetham and Jesse Capecelatro, University of Michigan

9:20 – 9:40 AM **Homogeneously Sheared Particle-Laden Turbulence in Two-Way Coupled Eulerian-Eulerian and Eulerian-Lagrangian Simulations**
M. Houssem Kasbaoui, Arizona State University

9:40 – 10:00 AM **Particle Dispersion and Deposition in Inhomogeneous Turbulent Flows**
Amir A. Mofakham and Goodarz Ahmadi, Clarkson University

10:00 – 10:20 AM Break – Foyer F-H

Session 2: Chair – William Fullmer

10:20 – 10:40 AM **Modeling Drag Forces in Bubbling Fluidized Beds Based on Experimental Data Fitting and Bubbling EMMS Model**
Daniel Kestering, Universidade do Vale do Rio dos Sinos

Tuesday, August 6, 2019 – Marriott at Waterfront Place – Salon E

10:40 – 11:00 AM **Drag Calculation Coupling with Clustering Phenomenon for Gas-solid Circulating Fluidized Bed Risers**
Zeneng Sun, Xiaoyang Wei, Chao Zhang, Jesse Zhu, University of Western Ontario

11:00 – 11:20 AM **Offline Evaluation of Agglomeration Tendency with a Gas-Solid Fluidized Bed of Identical Wet Particles: Model Development and Integration with MFiX**
Jaber Shabanian[1], Marc A. Duchesne[1], Allan Runstedtler[1], Madhava Syamlal[2], and Robin W. Hughes[1], [1]Natural Resources Canada, CanmetENERGY, [2]National Energy Technology Laboratory

11:20 – 11:40 AM **A Thermal Radiation Model for Numerical Simulation of Reacting Fluidized Beds with MFiX-TFM, MFiX-DEM and MFiX-PIC**
V M Krushnarao Kotteda, Michael Stoellinger, University of Wyoming

11:40 – 12:00 PM **Data-Driven Smart Proxy for Computational Fluid Mechanics**
Shahab D. Mohaghegh[1, 2], Mehrdad Shahnam[3], Ayodeji Aboaba[1], Yvon Martinez[1], Chris Guenther [3], Young Liu[3], Anthony Morrow[1], and Ashley Konya[1], [1]West Virginia University, [2]Intelligent Solutions, Inc., [3] National Energy Technology Laboratory

12:00 – 1:00 PM Lunch – Foyer F-H

Session 3: Chair – Mehrdad Shahnam

1:00 – 1:40 PM **Keynote Presentation: Gasification Research at Sotacarbo**
Andrea Porcu, Sotacarbo - Società Tecnologie Avanzate Carbone SpA

1:40 – 2:00 PM **Coal and Biomass Bubbling Fluidized Bed Gasifier - Design and Operation**
Ali Sivri, Amoolya Lalsare, Cosmin E. Dumitrescu, and Jianli Hu, West Virginia University

2:00 – 2:20 PM **Progress on Microwave Doppler Solids Flow Sensor Technology for Chemical Looping**
Benjamin Chorpening, Michael Spencer, Jared Charley, Sam Bayham, Douglas Straub, National Energy Technology Laboratory

2:20 – 2:40 PM **Hydrogen-Rich Syngas Production Through Synergistic Methane-Activated Catalytic Biomass Gasification**
Amoolya Lalsare, Yuxin Wang, Qingyuan Li, Ali Sivri, Roman J. Vukmanovich, Cosmin E. Dumitrescu, Jianli Hu, West Virginia University

2:40 – 3:00 PM Break – Foyer F-H

Tuesday, August 6, 2019 – Marriott at Waterfront Place – Salon E

Session 4: Chair – Jeff Dietiker

3:00 – 3:20 PM **Synchrotron X-ray Imaging for High-Speed Characterization of Multiphase Flows**
Theodore Heindel, Iowa State University

3:20 – 3:40 PM **Benchmarking CFD Simulation in Multiphase Systems Using Advanced Radioisotope and Non-radioisotope Measurement Techniques**
Binbin Qi, Omar Farid, and Muthanna H. Al-Dahhan, Missouri University of Science and Technology

3:40 – 4:00 PM **Euler-Euler Modelling and Validation of a Gas-Solid Fluidized Bed Using Advanced Measurement Techniques**
Sebastián Uribe, Muthanna Al-Dahhan, Missouri University of Science and Technology

4:00 – 4:20 PM **CFD-DEM Simulations of Proppant Particle Transport in Rough Walled Rock Fractures**
Amir A. Mofakham[1], Goodarz Ahmadi[1,2], and Dustin Crandall[2], [1]Clarkson University, [2]National Energy Technology Laboratory

4:20 – 4:40 PM **Some Accuracy Related Issues in Two-Fluid Hydrodynamic Sub-Grid Modeling of Gas-Solid Riser Flows**
Christian C. Milioli, Joseph Mouallem, Seyed R.A. Niaki, Norman Chavez-Cussy, Fernando E. Milioli, Universidade de São Paulo

4:40 – 5:00 PM **Multi-Scale Modelling and Simulation of Steam Reforming and Chemical Looping Reforming**
Juray De Wilde, Université Catholique de Louvain

5:00 PM Tuesday Session Ends

6:00 PM **Reception – Bourbon Prime Lounge –** *Pizza, snacks, cash bar*

Wednesday, August 7, 2019 – Marriott at Waterfront Place – Salon E

7:00 – 8:00 AM Continental Breakfast – Foyer F-H

8:00 AM **Reconvene**

Session 5: Chair – Mary Ann Clarke

8:00 – 8:20 AM **Influence of Operating Parameters on Mixing and Elutriation in Fluidized Bed Pyrolysis Reactors**
Zachary Mills[1], Liqiang Lu[2], Xi Gao[2], Gavin Wiggins[1], Charles Finney[1], Jim Parks[1], [1]Oak Ridge National Laboratory, [2]National Energy Technology Laboratory

8:20 – 8:40 AM **Computational Study on Biomass Fast Pyrolysis: Hydrodynamic Effects in a Laboratory-Scale Fluidized Bed**
Emilio Ramirez[1,2], Charles Finney[1], Tingwen Li[3], Mehrdad Shahnam[4], C. Stuart Daw[1], [1]Oak Ridge National Laboratory, [2]University of Tennessee, [3]SABIC Americas, [4]National Energy Technology Laboratory

8:40 – 9:00 AM **CFD Simulation of Hydrodynamics, Heat Transfer, RTD, and Chemical Reaction in a Pilot-Scale Biomass Pyrolysis Vapor-Phase Upgrading (VPU) Reactor**
Xi Gao[1], Tingwen Li[2], Kristin Smith[3], Katherine Gaston[3], National Energy Technology Laboratory, [2] SABIC Americas, [3]National Renewable Energy Laboratory

9:00 – 9:20 AM **CFD Modeling of KiOR's Proprietary Catalytic Fast Pyrolysis Reactors Using Barracuda™**
Bruce Adkins, Oak Ridge National Laboratory

9:20 – 9:40 AM **Funding Opportunities in Multiphase Flow at the National Science Foundation**
William Olbricht, Particulate and Multiphase Processes, National Science Foundation

9:40 – 10:00 AM Break – Foyer F-H

Session 6: Chair – Subhodeep Banerjee

10:00 – 10:20 AM **DEM for Non-Spherical Particulate Systems**
Vivek Srinivasan and Danesh Tafti, Virginia Tech

10:20 – 10:40 AM **Direct Numerical Simulations of Flow Around Assemblies of Non-Spherical Particles**
Sathish Sanjeevi, TU Delft, National Energy Technology Laboratory

Wednesday, August 7, 2019 – Marriott at Waterfront Place – Salon E

10:40 – 11:00 PM **Fluid Forces in Aspect Ratio 10:1 Ellipsoidal Particle Suspensions**
Ze Cao and Danesh Tafti, Virginia Tech

11:00 – 11:20 AM **Direct Numerical Simulation of Spray Atomization in Realistic Gas Turbine Injectors**
Marios Soteriou, United Technologies Research Center

11:20 – 11:40 AM **Efficiently Modeling Primary Liquid Atomization using an Eulerian-Lagrangian Hybrid Model in ANSYS Fluent**
Muhammad Sami, Jochen Schuetze, Paul Hutchinson, and Shailesh Ozarkar, ANSYS Inc.

11:40 – 12:00 PM **On the Mechanisms of Hinze Scale Bubble Deformation and Breakup in Strong Turbulence**
Ashik Ullah Mohammad Masuk, Ashwanth Salibindla, Shiyong Tan, Rui Ni, Johns Hopkins University

12:00 – 1:00 PM Lunch – Foyer F-H

Session 7: Chair – Avinash Vaidheeswaran

1:00 – 1:20 PM **Advanced Measurement Techniques for The Validation of a Single-Pseudophase CFD Model to Predict the Thermal Behavior of Nanofluids**
Sebastián Uribe, Muthanna Al-Dahhan, Missouri University of Science and Technology

1:20 – 1:40 PM **How Fast Do Bubbles Rise in High Energy Turbulence?**
Ashwanth Salibindla, Ashik Masuk, Rui Ni, Johns Hopkins University

1:40 – 2:00 PM **Local Validation of TBR Hydrodynamics Using Advanced Measurement Techniques**
Sebastián Uribe, Muthanna Al-Dahhan, Missouri University of Science and Technology

2:00 – 2:20 PM **Reversibility of Granular Rotations and Translations Under Cyclic Compression**
Zackery A. Benson, Anton Peshkov, Michelle Girvan, Derek C. Richardson, Wolfgang Losert, University of Maryland

2:20 – 2:40 PM **CFD DEM Analysis of a Dry Powder Inhaler with Containerized MFIX On Cloud**
V. Kumar[1], V. Kotteda[1,2], A Bhadhan[1], [1]University of Texas El Paso, [2]University of Wyoming

2:40 – 3:00 PM Break – Foyer F-H

Wednesday, August 7, 2019 – Marriott at Waterfront Place – Salon E

Session 8: Chair – William Rogers

3:00 – 3:20 PM **Developing a High-Fidelity CFD Model for CO_2 Separation by Adsorption**
Subhodeep Banerjee, National Energy Technology Laboratory

3:20 – 3:40 AM **Simulation of Residence Time in Solid Flowing Down Over Horizontal Perforated Plates**
Daniel Kestering, George Bleyer, Thiago Aquino, Guilherme Santos, Universidade do Vale do Rio dos Sinos, Uniersidade Federal de Santa Catarina

3:40 – 4:00 AM **STEV: A Stabilized Explicit Variable-Load Solver with Machine Learning Acceleration for the Rapid Solution of Stiff Chemical Kinetics**
Kyle Buchheit, Opeoluwa Owoyele, Terry Jordan, Dirk Van Essendelft, National Energy Technology Laboratory

4:00 PM Technical Meeting End

2019 NETL Workshop on Multiphase Flow Science

Thursday, August 8, 2019 – Marriott at Waterfront Place – Salon E

7:00 – 8:00 AM	Continental Breakfast – Foyer F-H
8:00 – 8:10 AM	**Welcome to the NETL Multiphase Flow Science Session** *William Rogers,* National Energy Technology Laboratory
8:10 – 8:40 AM	**MFiX and Exascale Computing – Development Update** *Jordan Musser*, National Energy Technology Laboratory
8:40 – 9:40 AM	**MFiX Suite Development Update** *Jeff Dietiker,* National Energy Technology Laboratory
9:40 – 10:00 AM	Break
10:00 – 10:45 AM	**MFiX Suite Quality Assurance Program** *Avinash Vaidheeswaran,* National Energy Technology Laboratory
10:45 – 11:30 PM	**Nodeworks: Optimization Toolset and Uncertainty Quantification Toolset** *Justin Weber, William Fullmer, Aytekin Gel,* National Energy Technology Laboratory
11:30 – 12:00 PM	**Tracker, an Opensource Particle Tracking Velocimetry Application Applied to Multiphase Flow Reactors** *Justin Weber, Michael Bobek, Steven Rowan, Jingsi Yang, Ronald Breault,* National Energy Technology Laboratory
12:00 – 1:00 PM	End of Workshop and Lunch – Foyer F-H

Posters

The Center for Multiphase Flow Research and Education (CoMFRE)
Theodore Heindel, Iowa State University

A Fluid-Consumption-Based Particle Transport Efficiency
Zhifeng Zhang, Antoine Pruvot, Pablo Cisternas, And James McAndrew, Air Liquide

Stuart Daw, age 69, passed away on July 2, 2019 after a 12+ year battle with cancer.

He is preceded in death by his father, Charles Edward Daw and survived by his wife Dianna Lynn Daw, mother Mildred Louise Daw, brother Murray Daw, step-daughters Robyn Norris and Amy Noe Howard, and nieces and nephews. He held a PhD from the University of Tennessee in Chemical Engineering and was a pioneer in his fields of interest - holding a number of patents with ORNL and having authored or co-authored more than 200 scientific papers and mentored dozens of PhD students around the world.

He was a founding member of Farragut Presbyterian Church, a Corporate Fellow with UT-Battelle (Oak Ridge National Laboratory), and a Professor with the Bredesen Center at the University of Tennessee. His passions for exploration and generous spirit led to a life of teaching, examination, explanation in both his professional and his private life with notable contributions to chemical and mechanical engineering science, cave exploration and more.

In his professional career as a chemical engineer, Stuart was exceptionally impactful in the science, and remarkably generous in mentoring and helping many others. He earned a Bachelor of Science degree at the University of Florida in 1973, then began his career at E.I. DuPont de Nemours in New Johnsonville, Tennessee, where he worked on improving chemical reactors used in producing titanium dioxide, a commonly used product whitener.

In 1979, he joined the staff at Oak Ridge National Laboratory, where he worked for 37 years before retiring in 2016 as a Corporate Fellow (the top technical position). While at ORNL, he maintained a long relationship with the University of Tennessee, first receiving his PhD in 1985 and then spending decades in adjunct or joint faculty positions, guiding research, teaching, and mentoring students. His achievements and leadership led to his election to Fellow of the American Institute of Chemical Engineers in 2013.

Stuart's natural curiosity and intuition drove him to constantly learn about new directions in science and to apply them to problems benefitting society. He was an internationally recognized pioneer in the application of chaos theory and nonlinear dynamics to complex problems such as diagnosis and control of complex chemical reactor and combustion systems, in the latter, principally automotive engines and utility boilers. His work with Ford Motor Company led to the first application of chaos control to reduce unsteady operation and pollutant emissions in automotive engines, and he was the driving force behind a commercial flame-monitoring system to allow fossil power plants to burn more efficiently and cleanly.

Stuart believed in the value of building teams from different backgrounds to approach problems with an interdisciplinary perspective. He formed and led two highly regarded research consortia for the Department of Energy. The first, an industry-government-university effort to understand and reduce pollutant emissions from cars and trucks, formed over 20 years ago and is still going strong. The second is a coalition of national laboratories to improve the thermochemical

production of biofuels via improved computer models. In these efforts, he took care to value the contributions and needs of the partners.

Stuart was a gentle mentor, always offering encouragement and guidance, believing that even improbable pursuits can yield useful surprises. He guided the research of dozens of students and junior staff members, being generous and approachable as an advisor. He was also magnanimous in including others to help further their careers and personal development. Stuart was first a friend, then a scientist. His example has served as inspiration for many of his proteges to emulate as they continue his legacy.

Stuart's hobbies included hiking, cycling, attending story-telling events, and archaeology; he was also an expert flint-knapper. He particularly enjoyed caving, which he engaged in for over 50 years with strong interests in conservation, exploration, and scientific study. Active in the local East Tennessee Grotto of the National Speleological Society, he also co-led the Cave Research Foundation expedition at the Cumberland Gap National Historical Park; he was elected as a fellow in both the NSS and CRF in recognition of his contributions to the caving community. In these pursuits, he translated his love for learning, even in the smallest of discoveries, and love for team building to his fellow cavers.

John Stephen “Jack” Halow, 76 of Garards Fort, died Sunday, June 30, 2019 in Ruby Memorial Hospital, Morgantown, WV. He was born September 1, 1942 in Johnstown, a son of the late John D. and Helen Weber Halow. Jack graduated from Penn State and went on to get his Ph.D. in Chemical Engineering from Virginia Tech. He worked as a researcher at Exxon and then for over 25 years at the Department of Energy, at the National Energy Technology Lab in Morgantown, WV. Jack had many interests and talents. Those included astronomy, pottery, painting, gardening, fishing, rock tumbling, computer programming, blacksmithing, researching local history, winemaking, and spending time with his children and grandchildren, to name just a few. When he retired in his early 60's, Jack and his wife Maria moved to an old farmhouse in Garards Fort, PA. He planted apples, blueberries and grapes. He also spent time restoring the farmhouse, working on the farm, and enjoying hobbies old and new. His love of science and research continued into retirement. In his later years, he collaborated with other scientists, was an adjunct professor of Physical Chemistry at Waynesburg University, and was a consultant and researcher for Separation Design LLC. He is survived by Maria Sanders Halow, whom he married on June 13, 1964. Also surviving are four children, Jocelyne (Joe) Patten of McDonald, Jessica Halow (Andy Brucia) of Seattle, WA, Stephen Halow (Randi Swearingen) of Waynesburg, Alex (Andrea) Halow of Athens, GA; three grandchildren, Madeira Halow, Ethan Patten and Jack Halow; a brother, William Hallow of Annapolis. Deceased are five siblings, Sylvester Ritchey, Raymond Ritchey, Ruth Ritchey, Grace Summerville, and Elizabeth Pisarski.