BARRACUDA VIRTUAL REACTOR®

USERS' CONFERENCE

June 27–28, 2019

W Hotel – Lakeshore

Chicago, Illinois USA

Agenda

Thursday, June 27th

7:00 am	8:00 am	**Registration and Breakfast**	
8:00 am	8:15 am	***Welcome***	
		Peter Blaser	CPFD Software
8:15 am	8:40 am	***Computational Modeling in FCC Design and Troubleshooting***	
		Raj Singh	TechnipFMC
8:40 am	9:05 am	***Advances in Barracuda Simulations of TRI Steam Reformer***	
		Ravi Chandran	ThermoChem Recovery International
9:05 am	9:30 am	***Barracuda Modeling of Oil Sand Transport, Hydraulic Fracturing and Biomass Conversion in the Energy Industry***	
		Kuochen Tsai	Shell
9:30 am	9:55 am	***Modeling of a Vortexting Circulating Fluidized Bed (VCFB) for Process Intensification***	
		Justin Weber	US Department of Energy, NETL
9:55 am	10:15 am	**BREAK**	
10:15 am	10:40 am	***Usage of Barracuda Virtual Reactor in the Cement Industry***	
		Adlan Omer	aixprocess GmbH
10:40 am	11: 05 am	***Comparison of CFD Models in Predicting Fluidized Behavior in Geldart B Particles***	
		Sina Tebianian	IFP Energies Nouvelles
11:05 am	11:30 am	***FCC Stripper/Standpipe Case Study – Off-Design Performance for Low Fines Catalyst***	
		Peter Loezos and Bryan Tomsula	CPFD Software
11:30 am	11:55 am	***Three Dimensional Full-Loop Simulation of Cold Gas-Solid Flow in Pilot-Scale Dual Fluidized Bed System***	
		Frederik Zafiryadis	Haldor Topsøe / Technical University of Denmark

Thursday, June 27th

11:55 am	12:20 pm	***1D and 3D Numerical Simulations of a 100kWth Coal CFB Combustor***
		Changwon Yang — University of Science & Technology, Korea
12:20 pm	1:20 pm	**LUNCH**
1:20 pm	1:40 pm	***CPFD 2.0***
		Rajat Barua — CPFD Software
1:40 pm	2:05 pm	***How PSRI Streamlines our Work Process using Barracuda Virtual Reactor***
		Ray Cocco — Particulate Solid Research, Inc.
2:05 pm	2:30 pm	***CFD Model Optimization for Simulation of Segregation in a Fluidized Bed of Particles with Different Sizes and Densities***
		Alex Kokourine — Hatch
2:30 pm	2:40 pm	***Introduction to CPFD Software Development***
		James Parker — CPFD Software
2:40 pm	3:05 pm	***Reduced Chemical Mechanism for Chemical Looping Combustion System***
		Hong-Shig Shim — Reaction Engineering International
3:05 pm	3:30 pm	***Acceleration of Stiff Chemistry Through TensorFlow and Machine Learning***
		Dirk Van Essendelft — US Department of Energy, NETL
3:30 pm	3:50 pm	**BREAK**
3:50 pm	4:10 pm	***Development Update: What's New and What's Coming***
		James Parker — CPFD Software
4:10 pm	4:35 pm	***Introducing Tecplot for Barracuda***
		Scott Fowler — Tecplot
4:35 pm	5:00 pm	***NVIDIA GPUs: What and Why***
		Reynaldo Gomez — NVIDIA
6:00 pm	9:00 pm	**Dinner and Reception at Museum of Contemporary Art**
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Agenda

Friday, June 28th

8:00 am	8:30 am	**BREAKFAST**
8:30 am	9:30 am	***Advanced Training: Recent Features, Output Analysis and Current Best Practices Part 1*** Bryan Tomsula — CPFD Software
9:30 am	9:45 am	**BREAK**
9:45 am	10:45 am	***Advanced Training: Recent Features, Output Analysis and Current Best Practices Part 2*** Ali Akhavan — CPFD Software
10:45 am	11:00 am	**BREAK**
11:00 am	12:00 pm	***Practical Deployment: Hardware, Operating Systems and Other Considerations*** Sam Clark — CPFD Software

Wi-Fi

Network: #BVRUC

Password: VirtualReactor

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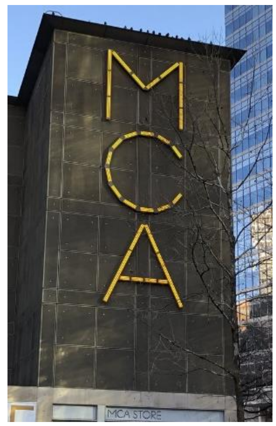
Museum of Contemporary Art



Please join us at the MCA for a Private Viewing, Cocktail Reception, and Dinner.

6:00 pm to 9:00 pm

Business Formal Attire Suggested

Walking directions from the W Hotel

Head North on Lake Shore Dr to E Chicago Ave. The MCA will be on the left. Please note, if driving there is a parking fee of $15.00 for the duration of the event.

Visit the museum website at mcachicago.org

Photography and Videography

The Museum has requested we respect the privacy of the artists. Please keep photos and videos of the art to a minimum.

Presentations

Computational Modeling in FCC Design and Troubleshooting

Raj Singh, Technip FMC

Computational modeling plays an increasingly important role in understanding gas and particle flow dynamics in the Fluid Catalytic Cracking (FCC) process, enabling refiners to consider low-risk and high value improvements to their FCCUs. TechnipFMC actively uses computational fluid dynamics (CFD) tools for FCC design optimization and for troubleshooting FCC operation. CFD provides adequate information required to understand and determine how hardware modifications and operational changes will impact gas-particle flow behavior and hence the overall performance of the unit. This paper discusses the significance of CFD modeling tools to effectively screen and evaluate new ideas and design changes, which improves existing technologies as well as the development of new ideas. Few case studies on revamp, hardware development and troubleshooting applications will be presented.

TechnipFMC

Raj has been with TechnipFMC for last 12 years, with total of 15 years of industrial experience. He has experience in FCC equipment design, technology development and troubleshooting and has contributed to a wide range of projects, including revamps, grassroots designs, process studies, CFD studies and FCC proposals. Raj has a MS in Chemical Engineering with specialization in the field of multiphase flow and fluidization from Illinois Institute of Technology, Chicago. He holds a Bachelor's degree in Chemical and Bio Engineering from Dr. B.R. Ambedkar Regional Engineering College, India.

Advances in Barracuda Simulations of TRI Stream Reformer

Ravi Chandran, ThermoChem Recovery International

TRI's steam reformer technology for carbonaceous feedstocks such as woody biomass, agricultural waste, Municipal Solid Waste (MSW), black liquor, waste sludge and young coals is characterized by indirect heating and deep bed fluidization in the bubbling regime. TRI has been actively working with CPFD since 2008 to model the steam reformer and validate the resulting Barracuda Virtual Reactor simulations. Many studies have been performed including, cold flow of single and multiple particle species, tube bundle representation, liquor injection, thermal and homogeneous/heterogeneous reaction modeling, solids mixing/segregation/entrainment, several different feedstocks, multiple reactor scales (laboratory to commercial) and first- and second-generation heater modes. Experimental and modeling insights have enhanced accuracy of predictions, while advances in both software and hardware have significantly reduced the total run time for quasi-steady convergence. Selected results from these studies will be presented.

TRI

Ravi has been on a quest to "minimize the increase in entropy" ever since he read the Feynman Lectures on Physics. Ravi is with TRI and leads technology development, scaleup and process modeling and is responsible for intellectual property. Previously, he was the Vice President of Engineering at Manufacturing and Technology Conversion International, Inc., Baltimore, Maryland and prior to that was Research Specialist at Babcock & Wilcox's R&D Division in Alliance, Ohio.

Barracuda Virtual Reactor Modeling of Oil Sand Transport, Hydraulic Fracturing and Biomass Conversion in the Energy Industry

Kuochen Tsai, Shell

Modeling high concentration solids in fluid flow has always been challenging. Continuum models using kinetic theory is expensive and can be difficult to include particle size distribution (PSD). DEM model has the advantage of modeling particle collisions directly but can be computationally very expensive in practice. Some other efforts to mimic the success of MP-PIC (e.g. Barracuda®) approach often resulted in numerical inconsistency.

Barracuda's unique efficiency in modeling condense particular flows makes it a perfect candidate for many large-scale problems and enables the design and scale-up process possible for dense slurry flow applications, including oil sand transport and proppant transport in hydraulic fracturing. Also discussed is the modeling of biomass in a bubbling bed where smaller and lighter particles are fed into a bubbling bed with heavier particles, to be digested and cracked to produce hydrocarbons.

Erosion aspects of oil sand transport and their challenges will be discussed. The issues are mainly the near-wall behavior of the particles that can have unphysical lifting, rendering the results useless for predictive models. However, faster version after v15 alleviated the difficulties in finding a work-around. However, a general model was eventually developed using the Eulerian-Granular model, where a more consistent correlation can be extracted with the aid of Barracuda and experimental data from the lab and the field.

Hydraulic fracturing uses hard proppants (e.g. sand) to crack open shale reservoir fractures and maintain its conductivity (aka. permeability). The understanding of proppant distribution in the multi-fracture production zone is critical for enhanced production. It can also be used to help optimize the completion process that will results in better production rate overall.

Biomass conversion to hydrocarbon is one way to achieve a carbon neutral future. However, the yield and energy efficiency has been long standing issues that hinder its progress. Here we demonstrate an aspect that validates the particle concentration distribution of the smaller and lighter particles within a bubbling bed with heavier and larger particles using published data. The resulting particle collision model can be used for the performance prediction of a biomass cracking reactor.

Kuochen has spent 12 years with Shell as a SME in CFD modeling. Before joining Shell, he worked for the Dow Chemical Company at Freeport for 9 years in Engineering Sciences. His current interests are in multiphase flows, biomass processing, erosion, flow assisted corrosion and data sciences. Kuochen also has a Ph.D in mechanical engineering from SUNY Stony Brook.

Modeling of a Vortexting Circulating Fluidized Bed (VCFB) for Process Intensification

Justin Weber, US Department of Energy, National Energy Technology Laboratory

The US Department of Energy is interested in developing small modular coal gasification units to support niche markets including combined heat and power, stranded fuels, and remote applications. To support the development of these modular systems, the development of novel reactors are being pursued to shrink to size of the gasifier, providing intensification of the process. One such reactor being develop is the vortexing circulating fluidized bed (VCFB) which operates like a cyclone. Since the center of the vortex is at a lower pressure than at the wall, a recycle loop of both solids and gas can be driven.

This reactor configuration is being developed at the US Department of Energy's National Energy Technology Laboratory in Morgantown, WV. Computational modeling in Barracuda is being used to help predict and inform design decisions of an eventual reacting unit. However, before the model can be used, it needs to be calibrated to an experimental cold-flow unit to provide confidence that the model is capturing the physics of process. Instead of simply fishing for parameters that match the experiment, a statistical approach has been used. A design of experiments is constructed varying a set of model parameters. The models are run and post processed to develop a quantity of interest (QOI), comparing the experimental results to the modeling results. A surrogate model is constructed to represent the QOI. Sobol sensitivity analysis of the surrogate model is performed to identify the most influential parameters that affect the results. Finally, an optimization routine is used to find the minimum of the response surface, resulting in the best set of parameters that match the computational model to the experiment.

Now that the parameters of the computational model have been tuned to the experimental unit, it can be used to explore the design of the VCFB. A critical piece of the VCFB is the design of the solids and gas recycle. The experimental unit has had problems with the horizontals accumulating solids and clogging. Using the tuned model, two other recycle designs have been investigated including a 45 degree angled return and a 45 degree angled return with gas injection in the corner, Figure 1. These models predict that by angling the recycle and injecting gas into the corner avoids solids accumulation and clogging of the recycle. Future work will continue to exercise Barracuda to aid in the design of a reacting VCFB gasifier which will eventually be constructed and tested at the Energy's National Energy Technology Laboratory.

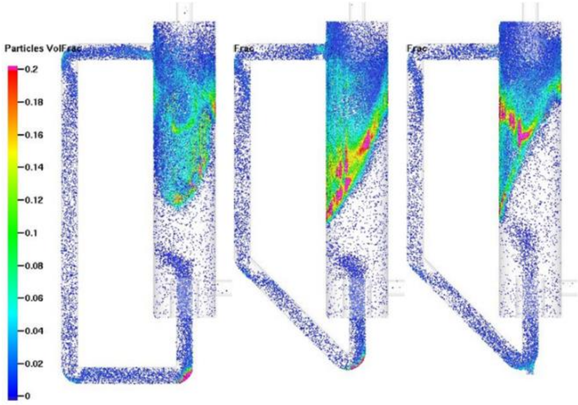


Figure 1:
Three solids recycle designs modeled with Barracuda.

Justin Weber received a BS in Mechanical Engineering from The Pennsylvania State University in 2009 and has been working at NETL since then. Justin is involved in numerous projects spread across both the computational and experimental domains with multiphase flow as a commonality. Current projects include development of MFIX, Nodeworks, Tracker, chemical looping combustion, gasification, and cold flow experimental measurement techniques including high-speed particle tracking and Electrical Capacitance Volume Tomography (ECVT).

Usage of Barracuda Virtual Reactor in the Cement Industry

Adlan Omer, aixprocess GmbH

Barracuda Virtual Reactor is especially powerful in applications in the Cement Industry, which we will demonstrate with multiple examples. However, the best outcomes are achieved when CFD is combined with broad knowledge of the industry in general, and deep knowledge of the equipment in particular. This presentation addresses questions such as: When should CFD be used? How to use CFD well? How to complement the CFD with other tools such as data mining and analytics? When to use CFD in-house versus consulting services from industry experts? In this presentation, we will try to shed light on these questions to maximize the benefit for users in the Cement Industry.

Adlan studied in Karlsruhe and Aachen power&process engineering and started in 2004 as a CFD engineer at aixprocess GmbH. A major focus for several years was, and still is, on modeling and consulting for clients with multiphase applications – especially in power generation and cement industry. After several positions within aixprocess Adlan is currently Key Account Manager, responsible for software sales and Senior Consultant.

Comparasion of CFD Models in Predicting Fluidized Behavior in Geldart B Particles

Sina Tebianian, IFP Energies Nouvelles

A particular flow regime occasionally observed when fluidizing Geldart B particles in small scale units is slugging. This flow regime, characterized by high pressure fluctuations and big bubbles that can cover the entire section of the fluidizing column (square-nosed slugs), may result in difficulty of extrapolation of the hydrodynamic results obtained for small units into larger scales.

CFD models represent a potential tool for the design of gas-fluidized beds. Despite the efforts of the scientific community, the ability of these models in predicting the hydrodynamic behavior of these multiphase systems is still limited. Robust and reliable CFD tools that can predict the hydrodynamics of group B particles slugging in lab or pilot scale units is extremely useful for beforehand definition of the operating conditions and geometry that can assure cold flow model experimentation reproducing the same hydrodynamics of large scale reactors.

In this work, two different commercial CFD tools have been compared in their ability of predicting hydrodynamic features of slugging gas-solid fluidized beds. The study is of special interest to chemical looping combustion process that employs Geldart B particles but also to fluidized bed combustion or gasification processes.

Different parameters such as bed expansion, pressure fluctuations, voidage and solid velocity obtained experimentally have been compared with CFD results and the effects of simulation parameters on the predicted flow structures have been discussed.

Dr. Sina Tebianian has obtained his PhD in fluidization at University of British Columbia under supervision of Prof. John Grace. Currently he is a research engineer at IFPEN responsible of design and scale-up of fluidization technologies such as Catalytic fast pyrolysis and Chemical Looping Combustion.

FCC Stripper/Standpipe Case Study – Off-Design Performance for Low Fines Catalyst

Peter Loezos and Bryan Tomsula, CPFD Software

The performance of FCCU strippers and standpipes is highly influenced by the Ecat PSD and/or fines content. When operating with a coarse Ecat or one that has a relatively low fines content, the catalyst can de-fluidize rapidly as it passes below the stripping steam ring resulting in significant stagnant or de-fluidized zones at the base of the stripper or conical transition to the standpipe. This de-fluidized catalyst can build up then erratically slump off into the standpipe, or bridge over the standpipe entry restricting flow. Once in the standpipe, the coarse or low fines content Ecat can de-fluidize rapidly between aeration taps resulting in stick-slip flow and excessive bubble formation depending on the extent of aeration and distance between aeration taps. The phenomena described above will result in unstable catalyst flow into the standpipe, low and erratic pressure build in the standpipe and ultimately unstable catalyst circulation in the FCCU.

When performing CFD simulations of stripper and standpipe flows, it is critical to capture the effect of catalyst PSD and fines content on the window of stable expansion and de-fluidization time to accurately capture the flow features of these systems. The physical parameters that captures these properties are readily extracted from simple experiments and can be inputted directly into Barracuda Virtual Reactor.

An example is presented from work done for a US Gulf Coast refiner operating with a relatively coarse Ecat. This refiner was experiencing unstable catalyst circulation and low/erratic DP across their spent catalyst standpipe and slide valve. Simple experiments were performed on a sample of the refiner's Ecat and the appropriate parameters were inputted into Barracuda Virtual Reactor. The base case performance of the FCCU stripper/standpipe was matched using Barracuda with no additional tuning. Stripper and standpipe performance were then modeled under the assumptions of a finer Ecat PSD and mechanical changes including modifications to the standpipe entry and fluffing steam ring to accommodate the refiner's current Ecat PSD.

Three Dimensional Full-loop Simulation of Cold Gas-Solid Flow in Pilot-Scale Dual Fluidized Bed System

Frederik Zafiryadis, Haldor Topsøe/Technical University of Denmark

Catalytic cracking of sugars in a circulating fluidized bed (CFB) system is a novel technology for producing intermediary oxygenate products that can be further converted to a variety of bio- based chemicals. The technology has the potential to enable economically and environmental sustainable production of bio-based chemicals.

The hydrodynamics of such a CFB system are very complex and play a critical role for successful operation of the plant. Hence, to support the design of the plant as well as the development and scaling-up of the technology, an in-depth understanding of the hydrodynamics in the system is needed. Three-dimensional computational particle fluid dynamics (CPFD) simulations are conducted based on the Eulerian-Lagrangian MP-PIC method to predict the hydrodynamic behavior of a cold flow-pilot scale CFB system at the Technical University of Denmark. The CFB system is of a dual fluidized bed (DFB) configuration, consisting of a reactor and a regenerator loop. Each loop is comprised of a riser, primary- and secondary cyclones, a bubbling bed, and a transfer line for connecting the two loops. A stripper section is located vertically below the regenerator bubbling bed to remove oxygen from the flow before re-entering the reactor riser. Detailed information on the hydrodynamic behavior of the system in terms of solids velocity, flux, residence time, as well as voidage and pressure distributions throughout the system are obtained and analyzed using a segregated modeling approach, decoupling the major parts of the system. The segregated method requires several subsystem simulations to be performed for achieving physical inflow conditions at the subsystem boundaries, improving modeling accuracy while reducing overall computational time and demands.

Technical University of Denmark DTU

Comparison of CPFD predictions with experimental data on the cold flow gas-solid pilot- scale model is conducted in terms of pressure distributions throughout the entire system, demonstrating the ability of the segregated full-loop model to capture the behavioral trends of the DFB system.

Further work includes modeling optimizations of each subsystem with respect to e.g. tuning of model parameters, drag modeling, grid- and sub-grid discretization. Further extensions of the model are to include a third (liquid) phase to simulate atomization and evaporation of the aqueous sugar solution required for ensuing introduction of chemical reactions to predict performance parameters (e.g conversion and yields) of the system in both pilot- and commercial- scale.

Frederik Zafiryadis holds a master's degree in mechanical engineering from the Technical University of Denmark (DTU), specializing in industrial fluid mechanics and computational fluid dynamics simulations of dilute particle-laden flow systems. He is experienced in experimental investigation of various types of flow phenomena; e.g. boundary layers, vortex-induced vibrations, and swirling flows, as well as numerical modeling of both internal and external, single- and multiphase flows using commercial and open-source CFD software. Since March 2019 he has been enrolled as a PhD student at the Chemical Engineering Department at DTU in collaboration with Haldor Topsøe, investigating and modeling the hydrodynamics of circulating fluidized beds, while undertaking short-termed consultancy projects as fluid mechanics specialist at the Danish engineering consultancy, Aerotak.

1D and 3D Numerical Simulations of a 100kWth Coal CFB Combustor

Changwon Yang, University of Science and Technology, Korea

In this presentation, the hydrodynamics and combustion characteristics of a 100kWth CFB combustor were investigated with two different numerical simulation approaches. IEA-FBC model and Computational Particle Fluid Dynamics (CPFD) software Barracuda were used for 1D and 3D simulation respectively. For 1D simulation, correlations for estimating axial solid hold up are necessary and they are dependent on the dimension of reactor, particle properties, and operating conditions. In the previous works, it was difficult to accurately predict the hydrodynamic characteristics of a CFB system since the correlations were obtained from limited experimental results. In this study, the solids decay constants obtained from 3D simulation results were used for 1D simulation, and the performance of 1D simulation was evaluated in comparison with the experiments and 3D simulation results.

Changwon Yang is a PhD student in green process and system engineering at University of science and technology. He is interested in design and fluid-dynamic analysis of a fluidized bed reactor system for gasification and combustion. His current research focuses on the simulation of the lateral and vertical solid hold-up distribution in a circulating fluidized bed combustor.

How PSRI Streamlines our Work Process Using Barracuda Virtual Reactor

Ray Cocco, Particulate Solid Research, Inc.

At PSRI, we use modeling to support and expand our experimental efforts and vice versa. CPFD's Barracuda Virtual Reactor is an essential part of that research process. PSRI performs experiments on a large scale with circulating fluidized beds up to 3-ft diameter riser and spans 90-ft in height, and fluidized beds ranging from 12-inch to 7-ft in diameter. With experiments on such a large scale, it would not be cost effective to proceed with a research program without first exploring our options using modeling. Similarly, modeling is an integral part of our analysis process. It helps us better understand what we are measuring and bridge that gap of what we can and cannot do in the lab. In short, modeling is used as our hypothesis, and as our analysis tool which driving our scientific method. Barracuda Virtual Reactor is an integral part of this approach. From the redesign of the PSRI attrition jet cup to understanding gas bypassing to reducing the number of experiments with our stripper study, Barracuda Virtual Reactor has streamlined our efforts while enriching our understanding and enhancing our technology.

Ray Cocco has been with PSRI for 13 years where he currently has the role of President and CEO. PSRI is a consortium-based company with 30 member companies headquartered in Canada, France, Finland, Germany, India, South Africa, Saudi Arabia and the United States. Before PSRI, Ray spend 17 years with The Dow Chemical Company where he led research and development efforts in numerous particle technology platforms including the production of WoodStalkTM (a particleboard made of straw) for Dow BioProducts, the production of vinyl chloride monomer and RCl oxidation using fluidized beds, the production of hydrocarbon using circulating fluidized beds, the development of polyolefin catalyst for fluidized beds, and in the production of aluminum nitride and silicon carbide ceramic powders using moving bed reactors.

In addition, Dr. Cocco was instrumental in bring in computational fluid dynamics, Six Sigma and Design for Six Sigma methodologies into Dow's research environment. Today, he is a board member of the University of Florida Chemical Engineering Advisory Board, Auburn University Chemical Engineering Advisory Board, University College at London's CNIE, and on the editorial boards for Powder and Bulk Engineering and Powder Technology. Ray was the past chair of the AIChE Particle Technology Forum (Group 3), past member of the AIChE Chemical Technology Operating Council (CTOC), and is currently an AIChE Fellow. Ray is also the past chairman of the World Congress in Particle Technology VIII in April 2018, He has 57 publications, three book chapters, several patents, numerous of invited presentations and consults for industry, national labs and universities on a regular basis.

CPFD Model Optimization for Simulation of Segregation in a Fluidized Bed of Particles with Different Sizes and Densities

Alex Kokourine, HATCH

Many industrial fluidized beds comprise of mixtures of particles with different sizes and densities. In order to achieve uniform fluidization and avoid segregation, the particle feed sizes can be optimized versus the fluidizing velocity. Optimization for different operating scenarios can be achieved by CPFD modeling, if the modeling parameters are fine-tuned based on a proper set of experimental data. Here, reported test data trends of particle segregation are compared with multiple sets of CPFD models, to show that pertinent modeling can reasonably predict the actual behavior of solids mixture, under a range of velocities.

Alexandre (Alex) is a Mechanical Engineer with specialization in mechanical design, heat and mass transfer, fluid bed (FB) and gasification technologies, fluid mechanics, plasma physics, physical vapor deposition (PVD), chemical vapor deposition (CVD), plasma and carbonyl fine powders. Project engineering experience with implementation of metal refining and deposition processes. More than thirty years' experience in research and development, mechanical design (Solid Edge, Solid Works), experimental testing, analytical (MathCAD) and computational (FEA-ANSYS, CFD-ANSYS CFX, CPFD-Barracuda) modeling.

Reduced Chemical Mechanism for Chemical Looping Combustion Systems

Hong-Shig Shim, Reaction Engineering International

Gas-phase chemical reactions can be modeled with a detailed mechanism, which usually includes many chemical species and several hundred reversible elementary reactions. However, implementation of a detailed chemical mechanism into a CFD code is prohibitive from the standpoint of both computational time and memory. Thus, our approach is to develop a reduced description of the detailed chemistry and implement it into a CFD framework.

CPFD's Barracuda has been used to evaluate particle flow behavior and the related chemistry in a dense flow reactor such as chemical looping combustion system. In this effort, the reduced mechanism is developed under chemical looping combustion relevant temperature and pressure conditions and interfaced with Barracuda with CPFD's help. A detailed mechanism with 93 chemical species and 495 reversible elementary reactions was used to generate a reduced mechanism with 25 species that was found to give excellent agreement with detailed chemistry, with acceptable computational demands using CPFD's Barracuda implementation.

The details of the reduced mechanism development and testing results will be discussed in this presentation.

Dr. Shim has worked for over 20 years in the fields of energy and environment focusing on utilizations of coal, oil, gas, and biomass. He has built and managed various international projects such as ultra supercritical steam power plant design evaluation and simulator development, NOx control strategy evaluation, coal/biomass gasification kinetics, oxy-firing assessment to mitigate CO2 emission, and advanced tool development.

His Ph.D. research completed at Brown University investigated thermal annealing of coal char at high temperature and developed image processing algorithm and structure parameters for nanostructure of carbonaceous material including coal char, graphite, and soot.

Acceleration of Stiff Chemistry Through TensorFlow and Machine Learning

Dirk Van Essendelft, US Department of Energy, National Energy Technology Laboratory

NETL has developed a novel stabilized, explicit solver that is accelerated with Machine Learning (ML) and is releasing it as part of the Carbonaceous Chemistry for Computational Modeling (C3M) software package. The solver uses several stabilization techniques and a new methodology we are calling “logically convergent, variable load” to ensure that the solver functions at maximum efficiency on GPU hardware. Each cell is solved in parallel and can evolve at its own time step and is removed from the integrator as it reaches the end time. The stabilization techniques adjust the time step for each cell to extend the explicit capability to stiffer problems. Further, the thermodynamic calculations were replaced by ML representations for a nearly 10% net time savings.

We are exploring use of the Volta architecture for further acceleration on tensor cores. The solver was integrated in NETL’s MFiX and was demonstrated to be as much as 280 times faster depending on the circumstances and problem size relative to the current state of the art LSODA solver on CPU.

C3M users will be able to access the TensorFlow protobuf files for the solvers which contain both the defined chemistry and the solvers for use in any compatible application. NETL is seeking to transfer this technology and test it in other CFD codes and believes that CPFD Barracuda could be an ideal candidate for integration

Dirk Van Essendelft obtained a BSE in Chemical Engineering from Calvin College in 2003, a MSE in Chemical and Biochemical Engineering from University of California in 2005, Irvine, and a Ph.D. in Energy and Geo-Environmental Engineering from The Pennsylvania State University in 2008. He has work experience in the pharmaceuticals, carbon capture and storage, bio-energy conversion, gasification, and high-performance computing. His current research interests are in applied computational chemistry for large scale industrial modeling using super computers. He currently manages the development of the National Energy Technology Laboratory’s Carbonaceous Chemistry for Computational Modeling (C3M) software and is developing unique solutions that allow high fidelity modeling at low computational cost.

Introducing Tecplot for Barracuda

Scott Fowler, Tecplot

Scott Fowler, Product Manager at Tecplot, Inc., will introduce an exciting partnership between CPFD and Tecplot, Inc in which all Barracuda users will be given access to Tecplot 360's best in class post-processing.

As Tecplot's Product Manager, Scott sees things from a customers' perspective and is a natural problem solver. It's his job to understand where the CFD and application markets are going, gather customer feedback, and make sure Tecplot develops products to meet those needs. Scott naturally stepped into the Product Management role after his tenure as the lead product architect for both of the products he now manages. His 16 years at Tecplot coupled with his Bachelor of Science in Electrical Engineering from the University of Washington give Scott the technical savvy to help Tecplot thrive in the coming years.

NVIDIA GPUs: What and Why

Reynaldo Gomez, NVIDIA

Efficient simulations are critical to practical industrial deployment of Barracuda Virtual Reactor. In this presentation Reynaldo Gomez, Energy Account Manager at NVIDIA Corporation, provides an overview of GPU vs CPU computing capabilities and introduces the NVIDIA software stack. This talk provides an overview of improvements in GPU computing including utilization of the latest GPU technology in the cloud.

Reynaldo Gomez is a GPU computing specialist for machine learning / deep learning and high performance computing in the energy sector. Prior to joining NVIDIA he worked at WesternGeco and IBM. Reynaldo has a Bachelor of Science degree in nuclear physics from the University of Texas at Austin.

Team cpfd

Ali Akhavan, Fluidization Engineer

Ali is a Fluidization Engineer at CPFD Software, based in Houston, with 14 years' experience involving diverse applications including gasification, environmental, power plant, bio-refinery, and petrochemical. Fluidization is the commonality to Ali's rich domestic and international experience, contributing toward his unique ability to integrate R&D into CPFD's industry-focused engineering service offerings. Ali holds a PhD in Chemical Engineering from Monash University in Australia.

Rajat Barua, President and CEO

Rajat Barua is President and CEO of CPFD Software. He has over 20 years of industry experience in roles that span engineering, operations, finance, sales and marketing. Prior to his current role, he served as CEO of Senscient, Inc., a technology company at the forefront of innovation in the field of lasers and sensor research, development and commercialization. Prior to Senscient, Rajat was Vice President at Lime Rock Partners, a private equity firm. He began his career with Schlumberger, where he served as a field engineer in North Africa and offshore, in the Gulf of Mexico. Rajat is a chemical engineering graduate of McGill University and holds an MBA degree from Harvard University.

Peter Blaser, Vice President of Engineering Services

Peter is Vice President of Engineering Services at CPFD Software with 20 years' experience developing and applying various general and specialized computational fluid dynamics (CFD) technologies. Since 2010 Peter has increasingly focused on refinery trouble-shooting and improvements via simulation, with particular emphasis on the FCCU and related components.

Peter began working with CFD at the University of Toronto, where he earned a Master's of Applied Science degree. Before joining CFPD in 2003, Peter worked for the CD-adapco group (now part of Siemens) deploying general purpose CFD technology across diverse industries.

Sam Clark, Senior Project Engineer

Sam is a Senior Project Engineer at CPFD with 14 years' experience modeling a wide range of industrial processes with CFD and CPFD software packages. He is an expert at modeling thermal, reacting, multiphase gas-particles systems with Barracuda Virtual Reactor. In addition to commercial simulation projects, Sam provides technical support to CPFD's global user base with excellence, leads in content development for software documentation, oversees our training programs and is a critical liaison between CPFD's engineering and development teams. Sam holds a Master of Science degree in Chemical Engineering from the University of New Mexico.

Miranda Fischer, Human Resources and Office Manager

Miranda is the Human Resources Manager and Office Manager at CPFD Software. After six years at the University of New Mexico as the Program Coordinator for Information Technology Program, Miranda began working at CPFD in 2011. She received her degree in Organizational Communication and Business Management. Over the years, her role has grown within the company and she began taking on additional projects which include marketing, logistics for events, and international trade show coordination. She also oversees all accounting and a variety of marketing functions for the company.

Paul Gomez, Customer Sales and Support Manager

Paul is CPFD Software's Customer Sales and Customer Support Manager with 15 years' experience in customer-facing support and leadership positions. Prior to joining CPFD Software in 2015, Paul held customer support, quality analyst, risk management, and investment services positions at Bank of America and Morgan Stanley. Paul is passionate about serving our customers with diligence and integrity, and bridges the gap between technical and commercial support activities. Paul holds a Bachelor of Science degree from the University of New Mexico.

Peter Loezos, Vice President of Operations

Peter is the Vice President of Operations, with 18 years of experience in the development and commercialization of new processes for the refining and petrochemical industries. His previous experience includes technology development roles in ExxonMobil, SABIC and Lummus Technology where he had a specific emphasis on fluidization engineering. Peter has a PhD in Chemical Engineering from Princeton University where his research included the development of CFD sub-grid models for gas-particle flow applications.

James Parker, Chief Technology Officer

James Parker, PhD, oversees the software development of Barracuda Virtual Reactor and CPFD's computational research of multiphase modeling techniques. Prior to his appointment as CTO, Dr. Parker was Principal Chemical Engineer for CPFD Software and used Barracuda Virtual Reactor on a wide range of fluidization modeling projects for refining, polyolefin, biomass, coal, and polysilicon applications. Dr. Parker received his PhD in Chemical Engineering from Oregon State University.

Bryan Tomsula, Technology Manager

Bryan Tomsula serves as Technology Manager for CPFD Software with 10 years of experience in the refining and petrochemical industries. His focus to date has been in various technology development, scale-up and licensing roles in the fields of fluid catalytic cracking, hydroprocessing and gasification. Bryan holds a BS degree from the University of Colorado in Chemical and Biological Engineering.

Survey

Please take a few moments and scan the QR Code below or visit the website to complete the conference survey.

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cpfd-software.com/survery2019

Thank You

We appreciate your time and we are grateful you could be part of this event. We look forward to our next conference.

Attendees

Attendee	Company
Berthod, Mikael	Abu Dhabi National Oil Company
Rakib, Mohammad	Abu Dhabi National Oil Company
Omer, Adlan	aixprocess GmbH
Avery, Clifford	Albemarle Corporation
Huang, Yanfen	Beijing Hi-Key Technology Company
Xuan, Harry	Beijing Hi-Key Technology Company
Ying, Liu	Beijing Hi-Key Technology Company
Venuturumilli, Raj	BP
Marquez, Carlos	CEMEX
Xiao, Hongliang	China University of Petroleum
Irikura, Motoki	Chiyoda Corporation
Reiling, Vince	Cornerstone Chemical Company
Miyamoto, Iori	CPFD Lab, Japan
Miyamoto, Yoshihiro	CPFD Lab, Japan
Dhodapkar, Shrikant	Dow Chemical
Yuan, Quan	Dow Chemical
Molnar, Michael	Dow Silicones Corporation
Badiola, Carlo	Encina Chemicals
Costenbader, Charles	Encina Chemicals
Wissmiller, Derek	Gas Technology Institute
Sirdeshpande, Avinash	GreatPoint Energy
Zafiryadis, Frederik	Haldor Topsøe, TU Denmark
Kokourine, Alex	HATCH
Knutson, Corey	Hemlock Semiconductor
Korinda, Andrew	Hemlock Semiconductor
Seman, Chris	Hemlock Semiconductor
Froehle, Derek	Honeywell UOP
Kulprathipanja, Sid	Honeywell UOP
Kaneko, Yasunobu	Idemitsu Kosan Co.
Amblard, Benjamin	IFP Energies Nouvelles
Tebianian, Sina	IFP Energies Nouvelles
Esmaeili Rad, Farnaz	Illinois Institute of Technology
Talmadge, Michael	Johnson Matthey

Attendee	Company
Kim, Hyesoo	Korea Institute of Industrial Technology
Kim, Youngdoo	Korea Institute of Industrial Technology
Yang, Changwon	Korea Institute of Industrial Technology
Jang, Gichan	Kyung-Won Tech
Kook, Jinwoo	Kyung-Won Tech
Lee, Doyong	Kyung-Won Tech
Seo, Kwangwon	Kyung-Won Tech
Chen, Liang	McDermott Lummus Technology
Liu, Zan	McDermott Lummus Technology
Wardinsky, Michael	Motiva Enterprises
Shabanian, Jaber	Natural Resources Canada, CanmetENERGY
Gomez, Reynaldo	NVIDIA
Monterosso, Federico	OMIQ srl
Cocco, Ray	Particulate Solid Research, Inc.
Ellis, Ryan	Particulate Solid Research, Inc.
Freireich, Ben	Particulate Solid Research, Inc.
Hankosky, Matt	Particulate Solid Research, Inc.
Issangya, Allan	Particulate Solid Research, Inc.
Karri, S.B. Reddy	Particulate Solid Research, Inc.
Kirkpatrick, Evan	Particulate Solid Research, Inc.
Knowlton, Ted	Particulate Solid Research, Inc.
LaMarche, Casey	Particulate Solid Research, Inc.
Sundaram, Shyam	Particulate Solid Research, Inc.
Afessa, Million Merid	Politecnico di Milano
Mossissa, Henok	Politecnico di Milano
Nega, Derese	Politecnico di Milano
Shim, Hong-Shig	Reaction Engineering International
Narayan, Raghu	Saudi Aramco
Tsai, Kouchen	Shell
Eagleson, Gary	TechnipFMC
Golczynski, Scott	TechnipFMC
Singh, Raj	TechnipFMC
Fowler, Scott	Tecplot
Chandran, Ravi	ThermoChem Recovery International
Massey, Ralph	Tronox
Bandara, Janitha	University of South-Eastern Norway
Van Essendelft, Dirk	US Department of Energy, NETL
Weber, Justin	US Department of Energy, NETL
Arshad, Ali	Vortex Oil Engineering S.A.

Notes

BARRACUDA VIRTUAL REACTOR®

FLUIDIZATION SIMULATION

SOFTWARE & SERVICES

CPFD Software's Virtual Reactor™ software simulates fluid-particle hydrodynamics, thermal behavior and chemical reactions enabling you to optimize the design and operation of fluidized processes and equipment for diverse industries including oil & gas, petrochemicals, gasification, power generation, materials processing, and more. Applications include unit design, scale-up, reliability, troubleshooting, off-design performance, economics, regulatory compliance, next-gen technology development and more.

- ✓ Determine Root Cause
- ✓ Reduce Risk through Virtual Testing
- ✓ Identify Optimization Opportunities
- ✓ Obtain Operational Readiness through Digital Assets