

The oil & gas industry faces many challenges from the onset of exploration to production of petroleum and natural gas, operating in extreme environments with increasing mandate to minimize CAPEX and OPEX, prioritize safety whilst reducing downtime and emissions. The role of advanced flow modeling technology is very important to overcome these challenges, especially during the current advancement in the digital era. Accurate digital representation of the upstream and downstream operations requires a multidisciplinary approach ranging from simple correlations to high-fidelity numerical analysis, such as Computational Fluid Dynamics (CFD). Scope and need for CFD modeling have gained significant momentum within the industry and growing rapidly, offering the opportunity to maximize innovation and engineering output at reduced time and cost.

Mission of the SPE-GCS Computational Fluid Dynamics Study Group to is to provide a common platform for CFD practitioners in Oil & Gas industry to foster knowledge sharing and networking, facilitate discussions, education/learning/training and develop boarder consensus on best practices in the area of CFD modelling for applications including (but not limited to) Near wellbore reservoir modelling, Drilling and Completion, Flow Assurance, Process and Process Safety, Offshore and Deepwater, Refining and Petrochemicals...

This is the 1st annual event of CFD Study Group and aims to deliver information and insights on physics-based modelling and its integration with data science for practical solutions to fluid flow problems in Oil and Gas industry. It has an excellent agenda with impressive lineup of speakers representing different sectors of the industry, academia and software vendors. This symposium will further act as a venue for experts from industry and academia to share experiences and lessons learned.

Program Chair: Madhusuden Agrawal **Program Coordinators:** Kedar Deshpande, Mazdak Parsi, Gocha Chochua, Bharat Tulsyan, Uday Godse

https://www.spegcs.org/study-groups/computational-fluid-dynamics/

	AGENDA
7:00 AM – 7:45 AM	Registration / Breakfast
7:45 AM – 8:00 AM	Welcome / Introduction
8:00 AM – 8:30 AM •	<u>Keynote Talk:</u> Role of Science-Based Modelling in the Oil & Gas industry, and How Digital Technologies can Help, Samir Khanna, BP
8:30 AM – 10:00 AM • •	Session-1 Data Analytics and Machine Learning in Flow Assurance, Prabu Parthasarathy, Wood Plc Simulation-Driven Design of Cyclone Type Autonomous Inflow Control Device for Water and Gas Control, Gocha Chochua, Schlumberger Accelerating Innovation in New Energies: Applications of Computational Methods, Santhosh Shankar, Shell Advances in CFD Modelling of Multi-Regime Multiphase Flows, Simon Lo, Siemens PLM Software
10:00 AM – 10:15 AM	Coffee Break
10:15 AM – noon • • •	Session-2 Keys to Particulate Diverter Applications: From CFD Modeling to Geomechanical Simulation, Jian Huang, Weatherford Choosing the Right Scale for Building Effective Digital Twins in Process Industries, Nandakumar, Louisiana State University Simulation-Based Digital Twins for Improved Asset Operation and Maintenance Management, Anchal Jatale, ANSYS CFD Modeling in Downhole Completion Tool Applications, Bin Zhu, Baker Modeling Polydisperse Multiphase Flows with Quadrature-Based Moment Methods in OpenQBMM, Alberto Passalacqua and Rodney Fox, Iowa State University
noon – 1:00 PM	Lunch Break
1:00 PM – 2:45 PM • • •	Session-3 A CFD Based Neural Network Model for Oil/Water Separation in Horizontal Pipelines, Kuochen Tsai, Shell Role of CFD Modelling in Digital Twin Concept for the Oil and Gas Industry, Ali Marzban, NOV Structural Integrity: Why Should I Care About Fluid Flow Simulation, Matt Straw, Norton Straw Consultants Multiphase Computational Fluid Dynamics at Exascale, Madhava Syamlal and William Rogers, NETL Assessment of Erosion in the Pipelines using Data Science, Erosion Science and CFD Methods, Praveen Gonuguntla and Damodaran Vedapuri, Tridiagonal
2:45 PM – 3:00 PM	Coffee Break
3:00 PM – 4:50 PM • • •	Session-4 Hybrid Digital Twin: The Challenges in Combining Data-Driven and Physics-based Techniques for Digital Twin Creation & Modeling, Srinath Madasu, Halliburton CFD – DEM Coupling for Modeling of Fluid Flow with Accurate Particle Representation, Marcus Reis and Clovis Maliska, ESSS Examples of Multiphysics Simulations and Predictive Analytics for Petroleum Engineering Applications, Mayank Tyagi, Louisiana State University Pragmatic Approach to Model Industrial Scale Gas-solids Reacting Flows, Sreekanth Pannala, SABIC Advanced CFD Modeling Tools to Accurately and Efficiently Predict Complex Hazardous Phenomena at

Role of Science-Based Modelling in the Oil & Gas industry, and How Digital Technologies can Help, Samir Khanna, BP

Abstract: Today, more than ever, computational and digital technologies play a critical role in the rapidly changing energy industry – challenged by the growing global demand under severe environmental constraints, and rigorous safety and financial demands under budget and time constraints. While science-based computational modelling has been a critical tool for addressing many of the industry's challenges, it still remains somewhat constrained on industrial-scale problems that are often multi-scale, multi-phase, and multi-physics. The biggest drawbacks of purely science-based modelling continue to be Accuracy & Speed. Although the oil & gas industry has been working closely with academia on addressing these limitations, the progress has been slow. Meanwhile, the industry has been recently introduced to enormous real-time data and digital technologies – AI/ML – that offer new opportunities to tackle some of the challenging operational issues. This purely data-driven approach also has its limitations – it only works in the regime in which the data was collected and does not necessarily provide the clear insights that a science-based approach provides for mitigating risks or optimizing production. The optimum path forward seems to be a hybrid approach – one that combines the strengths of both techniques to address our challenges more confidently and in a timely manner. The talk will briefly cover the current challenges and how a hybrid approach might help address them.

Speaker Bio: Samir joined BP in 2006 and is currently Research Advisor & Lead – Advanced Modelling Team in Group Research. His team provides technical support to the Group – in CFD, FEA, FSI & Multiphysics – and is responsible for developing enduring long-term capability in this technology and maximizing its value for BP. Samir received his PhD in Mechanical Engineering from the Pennsylvania State University in 1995 with a specialization in large-eddy-simulation (LES) of turbulent flows. This work was focused on accurate simulation and prediction of turbulent structures near flow boundaries. After Penn State, Samir worked at Corning Inc. for over 8 years, applying advanced mathematical modeling to various industrial processes used in making optical fibers for telecommunication, flat-panel glass for display, and ceramic-substrates for catalytic converters. Samir has 9 journal publications, 4 granted patents, and 2 published patent applications under consideration.

Data Analytics and Machine Learning in Flow Assurance, Prabu Parthasarathy, Wood Plc

Abstract: The democratization of machine learning and data analytics has thrown open a variety of new tools to the industry. These tools create new opportunities in the flow assurance area in both design studies and in operations phase. A few examples will be shown in this presentation demonstrating how these tools can be used ranging from reduction in study times to creating new methods of studying/troubleshooting difficult problems.

Speaker Bio: Prabu Parthasarathy is the VP of Intelligent Operations in Wood. Prabu completed his PhD in Mechanical Engineering and started at Wood in 2002 as a flow assurance engineer. He has led project teams in various phases of design in the US, Australia and India while expanding his role into operations and management. As the VP of intelligent Ops within Wood, Prabu looks after a portfolio of software products and services that deal with operational issues in the upstream, downstream, manufacturing and other industries as part of the Wood Automation and Control division. Intelligent Operations delivers its solutions globally and has been delivering solutions in the digital space for over 20 years. Prabu also serves as one of the digital leads within Wood.

<u>Simulation-Driven Design of Cyclone Type Autonomous Inflow Control Device for Water and Gas Control</u>, Gocha Chochua, Schlumberger

Abstract: Horizontal wells are considered superior to vertical and deviated wells because they increase reservoir contact; however, they can cone unwanted fluids (gas, water) causing reduced oil recovery and early well abandonment. Inflow Control Devices (ICDs) are typically installed along the completion string to delay coning and restrict water/gas influx. Once the coning occurs, conventional ICDs, such as channels and orifices, were found to be inadequate in choking back the unwanted fluids. Thus, new types of "autonomous" ICDs, or AICDs, were developed that choke back unwanted fluids more than conventional ICDs. Conversely, such AICDs have limitations related to bulkiness, moving parts, wellsite adjustability, flow performance predictability, and erosion. To overcome these limitations, a new AICD, operating on a principle of a cyclone, was developed by a synergy of the latest numerical technologies, such as Computational Fluid Dynamics (CFD) utilizing a high-fidelity Large Eddy Simulation (LES) turbulence model, and Design of Experiments (DOE) techniques. This CFD-driven design optimization involved utilization of highperformance computing (HPC) coupled with experimental validation. A DOE matrix of CFD analyses runs was performed to identify a geometry that would generate significantly higher pressure drop for water and gas than for oil. Early multiphase testing on a prototype device validated the concept, and CFD was used to improve the understanding of the operating principle and hence the design. CFD was further used to extrapolate the flow performance to a wider range of operating conditions. An expanded flow performance map and the use of non-dimensional parameters led to the development of a mechanistic AICD performance model which further enhanced our understanding of AICDs and allowed reservoir software programs to evaluate the production performance of wells with AICDs versus wells with conventional ICDs or no inflow control. The overall result is the new cyclonic AICD presented herein which is: 1) relatively compact, 2) without moving parts, 3) erosion resistant, 4) superior in multiphase performance, 5) easily adjustable at the wellsite with many settings, 6) accurately modeled with CFD, and 7) easy to incorporate into state-of-the-art reservoir simulation models.

Speaker Bio: Dr. Chochua has 17 years of experience in the Oil and Gas and Turbomachinery Industries. Early on in his career, Gocha obtained his Ph.D. degree in Aerospace Engineering from the University of Florida, specializing in Computational Fluid Dynamics. He worked as a Senior Aerodynamics Engineer at Siemens, developing new centrifugal compressors and separators. Gocha currently is a Principal Modeling and Simulation Engineer at a Technology Center of Schlumberger. His research interests include CFD, simulation-driven design, erosion modeling and mitigation, turbomachinery, thermal management, and multiphase flows. He has authored or co-authored 25 journal and conference publications and holds 20 granted and pending patents.

Accelerating Innovation in New Energies: Applications of Computational Methods, Santhosh Shankar, Shell

Abstract: Application of flow and transport models in the Oil and Gas industry have been immense- from upstream exploration, reservoir modeling, top-site design to midstream applications in flow assurance in pipelines modeling erosion and corrosion and assuring mechanical integrity and downstream applications in refining and chemicals. A unique opportunity presents itself today as many oil and gas majors are including as part of their portfolio, renewable, sustainable and green energy technology to provide cleaner energy options. Such technologies are currently in development stage and are expected to see scaled up deployment in the near future. Use of computational tools can help accelerate this development, allow for rapid prototyping and design optimization resulting in efficient technology maturation.

Speaker Bio: Santhosh Shankar is currently a scientist in the New Energy Research and Technology division's Long-Range Research Platform of Shell. His research interests include solar fuels, CO2-utilization, electro/photo catalytic pathways for fuel synthesis, and carbon capture. He currently leads the Carbon Capture program for dense energy carriers/solar fuels for Shell. Prior to this Santhosh worked in the Fluid Flow division carrying out research in multi-phase flows, fluid-structure interaction, turbulence and compressible flow modeling, and high-performance computing while supporting many upstream, midstream and downstream businesses in Shell. Santhosh graduated summa cum laude with a doctorate major in Aeronautical and Astronautical Engineering and minor in Mechanical Engineering from Stanford University, California, USA and a bachelor's degree from Indian Institute of Technology, Madras, India.

Advances in CFD Modelling of Multi-Regime Multiphase Flows, Simon Lo, Siemens PLM Software

Abstract: In this presentation we review the progress made in extending the Eulerian multiphase model in STAR-CCM+ to model multiple flow regimes in multiphase flows. New algorithms were derived to locate large scale interfaces and track their motions accurately. Important interface physics such as surface tension, surface damping on turbulence, interface heat and mass transfers can now be applied. The method is being extended to include film flow regime, and a novel approach to model phase-inversion based on the population balance method.

Speaker Bio: Simon Lo is a Director of Multiphase Model Development at Siemens Industry Software and since 2008 an Honorary Professor in Computational Multiphase Fluid Dynamics at The University of Nottingham UK. He received his PhD from Imperial College London in 1985. Since then he has been actively involved in the development of commercial CFD codes and their applications to industrial multiphase flows.

Keys to Particulate Diverter Applications: From CFD Modeling to Geomechanical Simulation, Jian Huang, Weatherford

Abstract: Currently, solid particulate diverters are frequently used for fluid stimulations, including fracturing, re-fracturing and acidizing. To ensure the success of a diversion operation, the most common strategy is increasing the usage of silica particles; however, this could lead to the excessive waste of particles and wellbore blockage. The success of these diversion treatments is truly dictated by the mechanical characteristics and wellbore displacement of the pumped solid diverters. A full understanding of the underlying mechanism of jamming and plugging can aid to design and pump the particulate diverters adequately. In this study, an integrated analysis is performed prior to a planned fracturing treatment to assess and improve the fluid diversion design. We proposed a workflow that combines analytical and numerical techniques to optimize the design of bi-particulate system, including flow rate, fluid viscosity, and particle size, shape, concentration, and ratio. Both a CFD-DEM model and a 3D fracture simulator are employed to model particle transport, fluid diversion and associated re-fracturing processes. Computational Fluid Dynamics / Discrete Element Method (CFD-DEM) models are used to model particle slurry transport during injection and successive plugging in the fluid diversion process. A 3D hydraulic fracture propagation simulator is utilized to simulate reservoir scale fracturing process. The code is advanced in modelling multi-physical processes involved in hydraulic fracture stimulation, including fracture height growth, stress shadows, and HF-NF interactions. This reservoir scale fracturing simulator can be customized for fluid diversion design analysis, when coupled with CFD-DEM models. Overall conductive reservoir volume and associated production is forecasted to compare different design scenarios under local reservoir and wellbore conditions. This workflow ensures effective and temporary isolation of existing openings by optimizing the bi-particulate diverting agent design, which enables target pressures to build-up behind the opening with minimal stimulation fluid leak. The workflow accounts for formation-specific properties and engineering designs that can be customized on a well-by-well basis. Based on the presented workflow, an integrated analysis has been conducted to quantify the influence of solid particle design on the jamming and plugging process and hence the diversion efficiency. From our analysis, engineered solid particulate diverters can seal the openings and build-up enough pressure to redirect fracturing fluid, as suggested from both the experiments and the numerical simulations. Non-engineered solid particles could fail in blocking the opening or cannot build sufficient pressure for effective diversion. By using the fit-for-purpose particle design, including size, ratio and concentration, the engineered solid particle diverter can effectively plug the active perforations and redistribute the fracturing fluid into nonactive perforations to creat additional fractures to boost production. According to our study, the particle design can be engineered properly to enhance the diversion efficiency and also optimize the usage of diverters. The presented design workflow and analysis will better enable us to design and customize solid particles for an efficient fluid diversion in both hydraulic fracturing and matrix acidizing operations.

Speaker Bio: Jian Huang is a Senior Geoscientist in the Department of Pressure Pumping Research & Development at Weatherford International. He has been with the company for six years. His research focuses on reservoir geomechanics, fracture mechanics, proppant placement, fluid diversion and reservoir simulation, which has already led to two granted U.S. patents and five other pending patent applications. Huang has authored or coauthored more than 30 technical papers. He holds a PhD degree in petroleum engineering from Texas A&M University.

<u>Choosing the Right Scale for Building Effective Digital Twins in Process Industries</u>, Nandakumar, Louisiana State University Abstract: The manufacturing technologies of the future for converting chemicals, materials, energy etc will be done in efficient, distributed, modular process equipment where multiphase flows are ubiquitous. Our traditional design approach has been to rely on rules of thumb, pilot

scale development and testing of process equipment which takes up to 20 years to develop a single technology. The design procedures are often highly empirical, dismissing the high degree of freedom that an engineer has at early stages of design by making ad-hoc design decisions, but pay the price during scale-up of processes through expensive pilot scale experiments. The question that I address in this presentation is "Can Advanced Computational modeling tools come to our rescue in minimizing the need for pilot scale experiments?" On the fundamental side, advanced algorithms for direct numerical simulation (DNS) and Discrete Particle Modelling (DPM) of multiphase flows aid in detailed understanding but for limited size. For dispersed rigid particles the Navier-Stokes equations are coupled with the rigid body dynamics in a rigorous fashion to track the particle motion in a fluid. These classes of algorithms show great promise in attempting to shed light on multiphase flows from which we can extract statistically meaningful average behavior for use in the design of large-scale engineering equipment. DNS simulations of controlled fluidparticle interactions in a shear flow are explored to learn about energy transfer in multiphase fluid-particle systems.

Speaker Bio: Dr. K. Nandakumar is currently Gordon A and Mary Cain Chair Professor at Louisiana State University. Prior to this he was the GASCO Chair Professor at The Petroleum Institute, Abu Dhabi. Formerly he was in the Department of Chemical and Materials Engineering at the University of Alberta, Edmonton, Canada for nearly 25 years. Dr. Nandakumar received his B. Tech from Madras University in 1973, M. Sc from University of Saskatchewan in 1975 and his PhD from Princeton University in 1979. He has received the Alexander von Humnboldt research fellowship from the German government in 1989-90 and the Albright & Wilson Americas Award from the Canadian Society of Chemical Engineering in 1991 for distinguished contributions to chemical engineering before reaching the age of 40. Dr. Nandakumar was elected as Fellow of the Chemical Institute of Canada in 1991 and a Fellow of the Engineering Institute of Canada in 2006 and Fellow of the Canadian Academy of Engineering in 2007. He has received, from the University of Alberta, the McCalla Professorship (1992), the Killam Annual professorship (2001) for excellence in research and the Rutherford Award (2001) for excellence in teaching. He has also received the Excellence in Education award (2002) from APEGGA, the professional engineering association in Alberta. He was Editor-in-Chief of The Canadian Journal of Chemical Engineering during 2005-2009. Dr. Nandakumar is also the recipient of the premier award of The Canadian Society for Chemical Engineering, called the R.S. Jane Memorial Award in 2008.

Simulation-Based Digital Twins for Improved Asset Operation and Maintenance Management, Anchal Jatale, ANSYS

Abstract: The insight of physics-based simulation in conjunction with advancement in collection and usage of sensor data enabled by the wireless technology and cloud computing has created great opportunities. It can drastically reduce risks associated with cost and schedule overruns resulted in less warranty cost and unexpected downtime. Simulation technology plays a central role in increasing the ROI related to IoT and digital-twins initiatives. It can provide insight from the deployment stage of the IoT platform to its operation and end of life. This includes sensor placement optimization to physics-based data interpretations and physics-based decision making. Additionally, it is being used for monitoring, diagnostics, prognostics, and prescriptive resolutions to optimize asset performance and utilization and record the digital footprint of the system. This technology also provides valuable insight for future product, system and subsystem requirements and design. This talk will share the vision and solutions for digitalization of assets/process using ANSYS platform. Relevant case studies with a comprehensive simulation ecosystem together with system-level modeling and Reduced order model approach will be covered.

Speaker Bio: Anchal Jatale, is currently serving as North America oil & gas industry lead for ANSYS. His background is in CFD modeling and has experience of 10+ years in modeling and simulations. For the past couple of years, he is spearheading ANSYS Digital twin engagements in O&G industry. His expertise is in Reduced order modeling, system modeling, reacting flow, combustion, multi-phase flow. Prior to joining ANSYS he received his doctorate in Chemical Engineering from University of Utah.

CFD Modeling in Downhole Completion Tool Applications, Bin Zhu, Baker

Abstract: CFD modeling is of great importance in understanding the physics related to downhole fluid flow, maintaining the safety of the downhole tools, as well as promoting oil and gas productivity. Two CFD related examples were discussed in this presentation. The first example is CFD erosion modeling for an x-annular flow valve (X-AFV), using a CFD erosion model developed at Baker Hughes. The model was first calibrated using elbow flow tested erosion results. The second one is about the same x-annular flow valve with high gas flow passing through the valve, causing pressure oscillation due to flow separation and high turbulence energy. The valve port region was identified as the primary vibration source. CFD was conducted on this part of the tool. Turbulent transient flow was modelled with Detached Eddy Simulation (DES) turbulence model. A Random Vibration Analysis (RVA) was utilized to obtain the PSD and root mean square of stresses to assess the random vibration effect, by using PSD of excitation pressure obtained from CFD prediction.

Speaker Bio: Bin Zhu, PhD in Mechanical Engineering from Tsinghua University, China. He joined Chinese Academy of Sciences as a research fellow after receiving his PhD degree in 1993. He then worked as a senior turbomachinery aerodynamic engineer in Beijing Full Three Dimension Energy Technology Co. Dr. Bin Zhu went to US in 1999 and had worked as a research scientist at Pennsylvanian State University, Michigan State University, and Iowa State University. He joined Husqvarna as a senior project engineer in 2006. In 2013, He joined Baker Hughes as a CFD/FEA Engineer. Dr. Bin Zhu's expertise is CFD/FEA modeling in aerospace, power and oil & gas industry.

<u>Modeling Polydisperse Multiphase Flows with Quadrature-Based Moment Methods in OpenQBMM</u>, Alberto Passalacqua and Rodney Fox, Iowa State University

Abstract: Polydisperse multiphase flows are encountered in a variety of applications of interest to the chemical, mechanical, pharmaceutical industry, where several products are obtained through the interaction and reaction of substances in gas, liquid and solid phase. Example applications involving these flows are the preparation of medications by means of precipitation, the formation of polluting particles in engines

and the production of certain polymeric materials. While these processes differ for the complex chemical reactions that lead to the products, and for the type of phases involved, they all fall into the category of polydisperse reacting flows, which includes flows where particles, bubbles or droplets are present in a main carrier phase, and form (nucleation), evolve (aggregation, breakup, growth) and react (combustion, ...). These flows can be described by means of a generalized population balance equation, whose unknown is a number density function (NDF) associated to the population of particles in the multi-phase flows. The solution of this equation is particularly challenging due to the number of independent variables of the problem, and the complexity of the physical phenomena that characterize these flows. An efficient approach to address these challenges are quadrature-based moment methods (QBMM), which track the spatiotemporal evolution of statistical quantities related to the NDF called moments. This approach will be illustrated during this lecture referring to example applications involving nanoparticle formations, gasliquid and gas-solid systems.

Speaker Bio: Alberto Passalacqua is associate professor of Mechanical Engineering at Iowa State University, with a courtesy appointment in Chemical and Biological Engineering. He is team leader for device scale numerical simulation in the Center for Multiphase Flow Research and Education (CoMFRE) at Iowa State University, and the lead developer of OpenQBMM, the first open-source implementation of quadrature-based moment methods into OpenFOAM. He was recipient of the American Chemical Society – Petroleum Research Fund Doctoral New Investigator award in 2014. He has received the Jean d'Alembert junior research fellowship at Université Paris-Saclay (France) in Summer 2017 and 2018. His research, funded by the US National Science Foundation and by the US Department of Energy, focuses on the development, implementation and validation of meso- and macro-scale computational models for reacting multiphase flows.

A CFD Based Neural Network Model for Oil/Water Separation in Horizontal Pipelines, Kuochen Tsai, Shell

Abstract: High fidelity 3-D engineering simulations are valuable tools providing recommendations and solutions difficult to obtain otherwise. However, those simulations can be costly due to expensive computational requirements. In this study, a deep neural network model trained by computational fluid dynamics simulations capable of predicting oi/water separation in horizontal oil pipelines was developed to accelerate and replace the CFD simulations. The goal is to provide useful information for oil production operators to effectively determine the use of corrosion inhibitors, which can add significant cost to the operation, and incorrect decisions can have serious impact on our environment. The CFD model was developed in the past 4 years for oil/water separation in horizontal pipelines to predict the water wetting probability on carbon steel pipeline surfaces. The model has been shown to correctly reproduce the flow regime map widely used in industry across ranges of water cut, mixture velocity, pipe diameter, oil density, viscosity and surface tension. However, the model requires expert set up and can take days to complete. Recently deep learning neural network algorithms has gaining momentum in the way that it automates the correlation construction between input and output data and allows complex hyper-dimensional correlations to be built with high accuracy. The efficiency comes from the optimization procedure unique to convolutional neural network (CNN) models. By parametrizing the CFD simulations it is possible to pre-calculate the results in all the necessary parametric spaces and use them to train the CNN model. The preliminary results in two parametric spaces, water cut and mixture velocity, are presented. The trained CNN model showed very high accuracy with the mean square errors lower than 0.01 in all cases. A total of ~4,000 data points were used to train the CNN model. The training time was around 4 minutes, and the inferencing time was less than 5 milliseconds, a performance gain of 106 in comparison to the CFD simulations. The model is being extended to include the other parameters aforementioned. It can also be extended to model other types of predictions as well, such as erosion and corrosion, and with more complex geometries other than straight pipes. The possibilities are endless.

Speaker Bio: 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 has a Ph.D in mechanical engineering from SUNY Stony Brook.

Role of CFD Modelling in Digital Twin Concept for the Oil and Gas Industry, Ali Marzban, NOV

Abstract: Computational Fluid Dynamics (CFD) has been a key solution to a lot of oil and gas industry problems before. Recently, implementation of CFD in digital twin concept has improved different product lines in terms of efficiency and life expectancy. During this presentation, some examples of digital twin concept in oil and gas industry will be presented.

Speaker Bio: Dr. Marzban has been involved in design and analysis of aviation and oil and gas products for more than ten years. His multidisciplinary background includes 3D linear/non-linear Finite Element (FE) and Computational Fluid Dynamics (CFD) analysis and design of major subsea products including XMass trees, Subsea Umbilical Termination Assembly (SUTA) boxes, Subsea Electronic Module (SEM), Subsea Control Module (SCM), subsea mudmat, Blowout Preventer (BOP), pumps, pipelines, pressure vessels, valves, jumpers and risers using DNV, NORSOK, API and ASME codes. He was also involved in structural/thermal and drop object analysis, fatigue and failure life calculations of various aviation components. He has extensive experience in performing advanced modeling, analysis and design.

Structural Integrity: Why Should I Care About Fluid Flow Simulation, Matt Straw, Norton Straw Consultants

Abstract: Structural integrity of a production or process system can be threatened both by the product flowing within a system and by the surrounding environment (whether wind, wave, current or temperature), often through complex fluid-structure interactions. In this presentation Norton Straw Consultants will present how our team approaches a range of engineering design and operational challenges, faced in oil and gas production and processing, where fluid flow simulation has been critical to understanding structural integrity and system performance. Examples provided will range from quantifying flow-induced vibration to understanding riser damage and the integrity of separator internals. The presentation will discuss how simulation approaches, such as computational fluid dynamics (CFD), finite element analysis (FEA) and system

simulation can be applied and combined to help find safe, practical and reliable engineering solutions to integrity challenges. Should time permit, a brief introduction will be given of Norton Straw's work in operational digital twins, using real-time data and physics-based simulation, to quantify and extend the life of complex engineering systems.

Speaker Bio: Dr Matt Straw works for Norton Straw, a specialist engineering and technology consultancy providing design and operational support as well as capability development and technology strategy services across a range of industries. Matt has over 20 years' experience in oil and gas in the application of engineering simulation and mathematical modelling to a wide range of design and operational challenges; including process and separation systems, subsea and flow assurance as well as process safety, artic operations and offshore engineering. Alongside technical work, Matt is actively helping to develop and implement strategies to maximize the value of engineering simulation and digital twins to support engineering design and operational activities.

Multiphase Computational Fluid Dynamics at Exascale, Madhava Syamlal and William Rogers, NETL

Abstract: The National Energy Technology Laboratory (NETL) has decades long history of developing and applying multiphase computational fluid dynamics models for trouble shooting and scaling up multiphase reactors used in fossil energy technologies. NETL maintains the open source, MFIX suite of multiphase computational fluid dynamics (CFD) codes that includes two-fluid model, discrete element model (DEM), and particle in cell (PIC) methods (https://mfix.netl.doe.gov/). MFIX has over 5,000 registered users world-wide and has been used at U.S. Department of Energy for reactor design and troubleshooting in fossil, bio, nuclear, and solar energy and nuclear waste treatment. The development of a version of the code called MFIX-Exa, which enables MFIX simulations on exascale computers, began in November 2016. This development project takes place under the Exascale Computing Project (ECP), established by US Department of Energy for accelerating delivery of a capable exascale computing ecosystem for breakthroughs in scientific discovery, energy assurance, economic competitiveness, and national security. The challenge problem of MFIX-Exa is to conduct a CFD-DEM simulation of a 50-kW chemical looping reactor at NETL, which will require tracking the five billion particles in the reactor, representing the full-loop reactor geometry, describing different gas-solids flow regimes occurring in the reactor, and including all relevant physicochemical phenomena.

Speaker Bio: Madhava Syamlal is Senior Fellow, Computational Engineering at National Energy Technology Laboratory (NETL). Dr. Syamlal is responsible for the development of computational science and engineering capability at NETL and for its applications to accelerate energy technology development. He also serves as the DOE Technical Director of NETL's University Coalition for Fossil Energy Research and leads an effort under the Exascale Computing Project. His degrees are in chemical engineering: B.Tech from IIT (BHU), and MS and PhD from IIT, Chicago. His significant accomplishments include advancing multiphase computational fluid dynamics (CFD) theory and numerical methods, developing the open-source multiphase CFD code MFIX, developing software for directly linking Aspen Plus and FLUENT simulations, and serving as the founding Technical Director of Carbon Capture Simulation Initiative that developed computational tools for accelerating the commercialization of carbon capture technologies. He is a fellow of AIChE and the recipient of numerous awards, including R&100 awards, DOE Secretary's Achievement Honor Award, and AIChE's Fluidization Process Recognition Award.

<u>Assessment of Erosion in the Pipelines using Data Science, Erosion Science and CFD Methods</u>, Praveen Gonuguntla and Damodaran Vedapuri, Tridiagonal

Abstract: Solid particle erosion is one of the principal modes of pipeline failures. A reliable prediction of erosion rates is imperative in the design and operation of oil and gas production facilities over the life of the field. There are four different approaches by which erosion in pipelines are studied/estimated in a field, and these are Lab and Field Scale Erosion Tests, CFD Models, Empirical Models and Data driven models. Lab/field scale erosion tests are an ideal model of erosion assessment. These are the accelerated erosion tests under control environment where similarity in pipeline configuration, velocities, particle size, MOC and GLR can be achieved, However, tests can be time consuming. Several empirical models are available for erosion estimation. The DNV model and the ECRC models are the most notable. Empirical models, models tend to vary by order of magnitude amongst themselves in their estimates of operational envelopes and it is important to understand their limitations when utilizing them. CFD modeling of Erosion has gained significant traction over the last decade. The predictive capabilities match closely with experiments in single phase systems. They also provide details on erosion hot spots. This is extremely critical when complex geometries need to be monitored. Data driven models in the last few years have gained significant interest in the industry. While the tools available for statistical analysis of large volumes of data have significantly advanced, key challenges stem from the quality of data and understanding of underlying science that governs a process. Data collection, cleansing, methods to deal with missing data are some of the key questions that need to be addressed. In this presentation, you will gain insights on how different empirical models and CFD models predict the erosion in pipelines. Pitfalls of these predictions and the variation in operational envelopes these models predict will be discussed. Also, the presentation will touch upon how a Data driven model framework

Speaker Bio: Praveen Gonuguntla is currently a Senior CFD Engineer at Tridiagonal Solutions Inc., based out in San Antonio. For the past ten years, he has performed extensive CFD analysis of Upstream and Downstream Oil&Gas applications. The experimental analysis in the field of erosion is another such area where he worked. He holds a master's degree in mechanical engineering. His areas of interest are erosion, optimization of downhole tool designs and refinery equipment, multiphase flows in oil & gas production systems and combustion modeling.

<u>Hybrid Digital Twin: The Challenges in Combining Data-Driven and Physics-based Techniques for Digital Twin Creation & Modeling,</u> Srinath Madasu, Halliburton

Abstract: The adoption of data-driven and/or physics-based reduced-order models as a digital twin in the aviation, aerospace, and renewable energy industries have experienced enormous benefits over the past decade. Benefits captured across these industries include: improved quality and speed of decision-making, greater asset utilization, condition-based monitoring and prognostication, enhanced operational-efficiency and improvements in preventive maintenance. Physics-based models in Computational Fluid Dynamics (CFD) are the main approach for simulation and prediction. However, these models suffer from inherent assumptions on which they are built. Moreover, key gaps exist in the understanding of basic principles concerning how and when to use different data-analytics tools to create a virtual representation from data, and then combining it with trusted physic-based modeling; thereby, allowing the assimilation and computational infrastructure, which in turn gives industries the opportunity to explore and take advantage of the exciting possibilities for digital twins to analyze physical assets efficiently and effectively. The challenge of creating these entities, either through physics-based methods, data-driven modelling or combining them to form a "hybrid digital twin," is of real interest to both academic and industry research and is the main motivation for this presentation.

Speaker Bio: Srinath Madasu is working as Technical Advisor at Halliburton. He did his Ph.D. from Drexel University, Philadelphia in Chemical Engineering in 2002. Srinath finished Post-Doctoral Research in Chemical engineering from The Pennsylvania State University, State College. He is working at Halliburton for 8 years after working at Maya Heat Transfer Technologies, Montreal as CFD and Heat Transfer Application Developer for 5 years. He received a MVP award in 2013 from Halliburton. His main interests are Machine Learning, Optimization, Robotics and Physics based Modeling. He developed real time machine learning and optimization model for drilling, artificial lift methods such as Gas lift and fracture cluster efficiency prediction. He has several patents, SPE; IEEE papers and journal publications.

<u>CFD – DEM Coupling for Modeling of Fluid Flow with Accurate Particle Representation</u>, Marcus Reis and Clovis Maliska, ESSS

Abstract: Particle laden flows are encountered in many industries including oil and gas, agroindustry, pharmaceutics, mining, and many others. Eulerian granular and Langrangian approaches in multiphase CFD are commonly used to model fluid-particle flows for some these applications. However multiphase CFD has limitations due to the lack of constitutive models that adequately describe the range of particle characteristics. The coupling between DEM and CFD is a promising approach and broadens the range of particle-fluid processes that can be handled with numerical simulation. This presentation will provide an overview and latest development of modelling approaches for the simulation of both dilute and dense-phase fluid-particle flows. In addition, the coupling approach for Rocky DEM and ANSYS FLUENT will be showcased, with few interesting applications examples for modeling complex flows where fluid details are needed and key interest involves model particle shape, particle break-up, separation, segregation and mixing.

Speaker Bio: Since ESSS beginning, in 1995, Marcus Reis has been involved with several activities at ESSS (a Latin America pioneer company in the field of numerical simulation). He started as software developer, but soon migrated to work with CFD consulting projects. As time went by, he has built a team of 70 technical specialists working with several disciplines in the field of computational modeling (CFD, FEA, EMAG, MDO and DEM). He has been involved with more than 100 projects for key customers in its territory among several industries segments, ranging from automotive, appliances and aerospace to mining and oil & gas. In parallel he also has initiated and developed the marketing and sales division of ESSS with a key focus on the global business development of Rocky DEM software. Marcus Reis has a M.Sc. and Mechanical Engineering degree from the Federal University of Santa Catarina where he was involved with the research on numerical heat transfer for aerospace applications. He also holds a MBA degree from Fundação Dom Cabral, Brazil.

<u>Examples of Multiphysics Simulations and Predictive Analytics for Petroleum Engineering Applications</u>, Mayank Tyagi, Louisiana State University

Abstract: Machine learning and predictive analytics based on complex data sets has shown great potential for finding insights in many fields. Petroleum engineering data sets can vary greatly in their size and types over the lifetime of a given asset. Typical exploration data sets would include seismic data, drilling data sets would include MWD data, reservoir management information would include decision based on simulations, and production data from multiple wells would include time series information on operations and possibly daily production rates. In this talk, several case studies from petroleum engineering to demonstrate the potential of predictive analytics in real-world applications. Examples include analysis of real field drilling data, reservoir simulation data, and well production data.

Speaker Bio: Prof. Mayank Tyagi is Chevron #3 designated associate professor at the Craft & Hawkins department of petroleum engineering, Louisiana State University (LSU). He also holds a joint faculty appointment at the Center for Computation & Technology (CCT), LSU since 2007. He obtained his Ph.D. in mechanical engineering from LSU and undergraduate in mechanical engineering from Indian Institute of Technology (IIT), Kanpur. His current research interests span across high performance computing (HPC) and data analytics for interdisciplinary petroleum engineering applications, image-based pore-scale modeling using lattice Boltzmann method (LBM), multiscale multiphase computational fluid dynamics (CFD), geothermal reservoir engineering, and unconventional reservoir simulations. He has also worked on the issues in the quantitative risk assessment (QRA) of offshore petroleum engineering operations and their impacts on regional economy. He has given numerous invited talks at India, China, and several US universities and published over fifty (50) peer-reviewed technical publications. He is an active member of university-industry consortium "Enabling Process Innovation through Computation (EPIC)" at LSU.

Pragmatic Approach to Model Industrial Scale Gas-solids Reacting Flows, Sreekanth Pannala, SABIC

Abstract: Developing new and efficient commercial scale multiphase reactors is extremely difficult as one needs to consider the complex interactions over a wide range of both temporal and spatial scales encountered in these systems (from molecules to macroscale). Therefore, it is

important to codify and automate the knowledge collectively acquired so far, reserving human resources for the creative solutions that build upon codifying past learnings. Computational science (algorithms, theory and modeling, computer science, etc.) combined with exponential growth in computing hardware has great potential to provide us valuable tools for improving the effectiveness of existing plants but also design new reactors. Industry is in desperate need of fast simulation tools that are comparable to the accuracy of the single-phase reacting flows to advance the adoption of multiphase flow reactors and primarily to reduce the risk of scale-up. On the other hand, academia and national laboratories are focused on improving numerical methods, submodels or certain physics to push the state-of-the-art and predictability of the models. However, there is tremendous need for rapid integration of various capabilities that exploit latest computer hardware improvements, robust model reduction techniques, etc. that would improve the computational tools available to the industry to deliver the next generation of efficient and cost-effective reactors. These developments typically fall into the valley of death where industry and software vendors feel these efforts are far-fetched while the academic world considers it incremental. One way to address this divide is to develop mechanistic upscaling framework to coarse-grain information from more detailed modeling approaches to fast models accessible to the industry with relatively minimal information loss. Presentation will include such an approach using a gas-phase fluidized bed polymerization reactor as an example. First, I will provide an overview of the various models currently used at the different scales in gas-solids reacting flows. The coupling across the scales will be introduced through few different approaches: a) Discrete-Continuum Coupling using Discrete Element Method for particles b) Upscaling data from Discrete Element Modeling results to continuum based Computational Fluid Dynamics (CFD) c) Upscaling information from CFD to simplified reactor network models. In conclusion, the presentation will elucidate the approaches and opportunities in bridging the gap between academic advances and industry needs to model and advance our understanding of gas-solids reacting flow reactors.

Speaker Bio: Dr. Sreekanth Pannala is a Research Fellow at SABIC from April 2015. Prior to this, he was a distinguished research staff member in the Computer Science and Mathematics Division at Oak Ridge National Laboratory. He received his B. Tech (1993) in Aerospace Engineering from IIT Kharagpur and M.S. (1994) and Ph.D. (2000) in Aerospace Engineering specializing in the area of computational combustion of two-phase flows from Georgia Tech. His expertise is primarily in the area of developing parallel algorithms and models for homogeneous and heterogeneous chemically reacting flows from device to micro scale. He received Federal Laboratory Technology Transfer award in 2006 and R&D 100 award in 2007 for his contribution to the development of MFIX (http://goo.gl/kOl30), an open-source multiphase reacting flows simulation suite. He has served as a principal investigator on various DOE computational science projects and has over 100 journal and conference publications in various areas of computational science and engineering. He also served as a lead editor for a book on computational gas-solids reacting flows (http://goo.gl/QwU32). He led the development of battery simulation software environment (http://batterysim.org). He was also awarded Secretary of Energy's Achievement Award - highest non-monetary award from Department of Energy.

Advanced CFD Modeling Tools to Accurately and Efficiently Predict Complex Hazardous Phenomena at Large-Scale Petrochemical Facilities, Drew Botwinick and Scott Davis, Gexcon US

Abstract: Resolving the combustion flow physics and chemistry of vapor cloud deflagrations in complex large-scale geometries, such as petrochemical facilities can be computationally challenging. Gexcon's software FLACS was created specifically to solve this problem and has been validated against thousands of deflagration experiments conducted at small, medium and large scales with fuels having a broad range of reactivity (mildly reactive, reactive, and extremely reactive). FLACS captures the effect of small obstacles while remaining computationally tractable by implementing a distributed porosity concept, thereby accurately representing confinement and congestion. Large geometries are modeled on a Cartesian grid with large objects represented on grid while smaller objects are resolved using sub-grid calculations of contribution to turbulence and flame folding. The drag from partially blocked cells is accounted for in the RANS equations through a modified turbulence generation rate term in the k-ɛ turbulence model. With this approach, sub-grid objects contribute to flow resistance and turbulence generation without needing to be fully resolved. This allows users to quickly simulate dispersion at large scales without excessive computational resources. In addition, FLACS uses a flamelet-based combustion model with one-step reaction kinetics characterized by the laminar burning velocity of the fuel-air mixture. Then, using the sub-grid models, the real flame area is properly described and corrected for curvature at smaller scales than the grid. FLACS accounts for flame acceleration due to flame instabilities, flame-folding by obstacles, and turbulent mixing. Accounting for these details is critical to accurately simulate explosion phenomena and provide an efficient way to simulate explosions at scales relevant to real facilities. Therefore, FLACS provides a practical computational environment to evaluate complex hazardous phenomena occurring at large-scale petrochemical facilities in an accurate, expedited and cos

Speaker Bio: Drew Botwinick is a Senior Risk Consultant at Gexcon US who performs risk assessments and process safety studies specializing in quantitative technical risk focused on fires and explosions, especially assessments involving extremely large or complex datasets. Drew has experience with various CFD packages including FLACS, KFX, and FDS as well as phenomenological models such as Phast. Drew has applied these to execute safety studies in various onshore and offshore contexts including onshore LNG liquefaction facilities, floating LNG facilities, FPSOs, and various types offshore platforms for different modes of operation including accounting for simultaneous operations (e.g. limited normal operations with simultaneous construction). Drew also has solid experience as a software engineer and systems architect for distributed computing systems. Drew's software development experience has facilitated analysis of extremely large and/or complex data sets. He has also developed multiple proprietary software products as well as tools to analyze various aspects of CFD simulations—from pre-processing to managing workloads to post-processing. In Drew's work, he has worked on a large variety of different situations—from simulating toxic gas dispersion across the entirety of a small island, to Monte Carlo-based evaluations of detonation prediction for a hydrogen-based facility, and even on evaluating the effects of methane produced from breaking down animal manure on fire and explosion risk in a closed building.