ANNUAL REPORT for the PIRE Project at City College of New York (2017-2022)

MULTI-SCALE, MULTI-PHASE PHENOMENA IN COMPLEX FLUIDS FOR THE ENERGY INDUSTRIES

Sponsored by the National Science Foundation

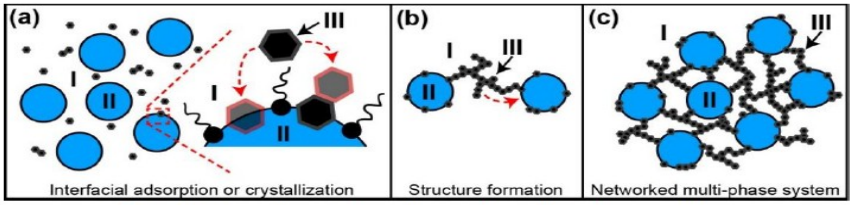
Prepared by

Masahiro Kawaji (Principal Investigator)

INTRODUCTION

A five-year, $5.2 million project supported by the National Science Foundation's Office of International Science & Engineering was launched in October, 2017 at the City College of New York (CCNY). This PIRE project builds upon and enhances existing collaborations among CCNY and three Norwegian, four French and five German institutions with the US playing a leadership role in investigations of multi-scale phenomena in complex (Non-Newtonian), multi-phase fluids that are vital to energy technologies. Multi-phase fluid flows play an important role in nature and in the environment. Multi-phase flow research is of vital importance to many key energy technologies on a global scale, including oil-gas production and processing, energy conversion and storage, refrigeration and heating/cooling industries, as well as mineral and materials processing, and the pharmaceutical, personal care and food industries.

This project will investigate phase and structure formation, molecular adsorption and reactions at and between interfaces as illustrated below, and their effect on macroscopic transport processes in complex multiphase systems.



Schematic of the Multi-scale, Multi-phase problem

The essential problem relates to the linkage of scales: strong coupling between molecular and macroscopic scales necessitates innovation in both experimental and modeling methods. Understanding of coupling between the molecular scale and the macroscale in such inherently multi-scale problems can enable control of properties of importance in many applications. Thus, this research project on complex fluids comprises of two research themes:

Research Theme #1. Molecular-scale phenomena in complex, multi-phase fluids: interfacial adsorption, reactions, and structure formation. The objective of this theme is to better understand: (i) molecular adsorption, crystal nucleation, and particle aggregation of the network-forming phase at interfaces, (ii) the subsequent formation of network structures by multi-layer adsorption, crystal growth, and particle aggregation within the continuous phase, and (iii) how to control these phenomena at a molecular level to eliminate, mitigate, promote, or accelerate network formation to optimize macroscopic fluid behavior.

Research Theme #2. Macroscopic complex fluid transport processes and properties: effects of interfacial and network structures. The objective of this theme is to quantitatively measure, understand, and control how network structures affect macroscopic transport and physicochemical properties of multi-phase complex fluids. The formation of interfacial and network structures is expected to affect phase stability, surface rheology, bulk rheology, phase distributions, sedimentation, and transport properties.

These themes are investigated under four Research Thrusts and Modeling & Simulation as explained in detail in the next section. The critical common issue is that molecular-scale phenomena, particularly at interfaces, impact macro-scale properties and behavior. The overarching research objectives of this PIRE project are thus to (i) elucidate molecular-level phenomena that govern the formation, aggregation and stability of interfaces and network structures in multi-phase systems, and (ii) control their development and effects on macro-scale rheology and transport processes.

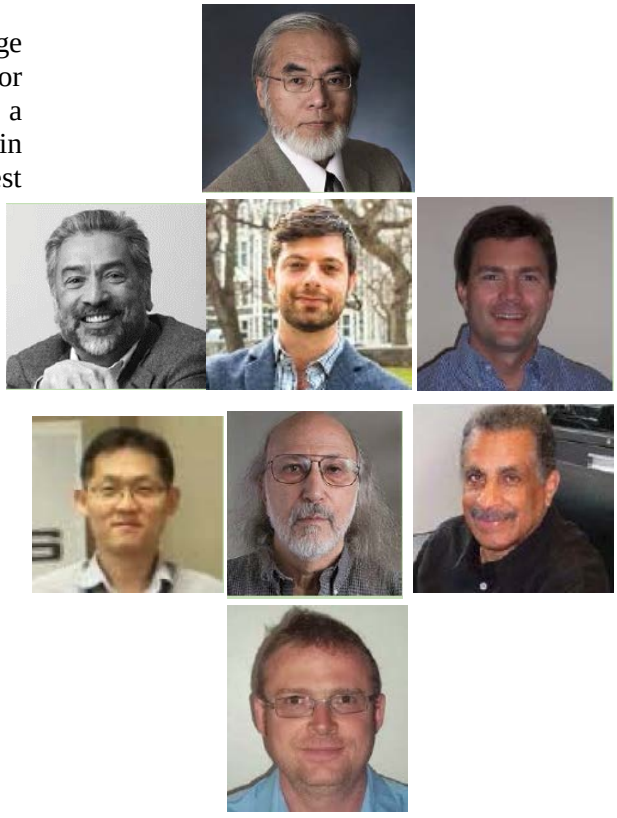
An important societal outcome of this project is that it would advance and transform key engineering technologies which are of high relevance in the energy industries and an important factor in environmental sustainability. The institutional impacts will result from the international partnership with some of the most respected international researchers in the field. The project is also intended to contribute to STEM education of exceptional undergraduate and graduate students from underrepresented groups by providing them with outstanding research opportunities and extensive international experiences at home and in partner countries.

International Collaborators and Their Funding Status

This project involves a total of twenty collaborating researchers (8 from Norway, 6 from France and 6 from Germany) from eleven institutions. Foreign sponsors of this international project include Norway's Research Council of Norway (RCN), France's Agence Nationale de la Recherche (ANR) and Germany's Deutsche Forschungsgemeinschaft (DFG). Norwegian collaborators applied to the PIRE program and received their funding in 2017. French collaborators have recently received approval for their funding request from ANR. German collaborators are yet to receive their grant from DFG in 2018-19.

PIRE Faculty at City College of New York

Six Engineering faculty and one Physics faculty at City College of New York are involved in this project as PI, Co-PI and Senior Personnel as listed below. Dr. Vincent Pauchard who was a faculty member at the start of this project but left CCNY in January, 2018, is still involved in this project as a guest researcher of the CUNY Energy Institute.



PI: Masahiro Kawaji (Prof. of Mechanical Engineering; Associate Director, CUNY Energy Institute)

Co-PI: Sanjoy Banerjee (Distinguished Prof. of Chemical Engineering; Director, CUNY Energy Institute)

Co-PI: Robert Messinger (Assistant Prof. of Chemical Engineering; CUNY Energy Institute)

Co-PI: Jeff Morris (Prof. of Chemical Engineering; Director Levich Institute)

Co-PI: Taehun Lee (Associate Prof. of Mechanical Engineering; CUNY Energy Institute)

Senior Personnel: Joel Koplik (Prof. of Physics; Levich Institute)

Senior Personnel: Charles Watkins (Prof. of Mechanical Engineering)

Guest Researcher: Dr. Vincent Pauchard

Postdoctoral Fellow

A postdoctoral researcher, Dr. Dinesh Kalaga, joined the PIRE project in March, 2018. He has a PhD in Chemical Engineering and has worked on multiphase reactors including a bubble column. At CCNY, he has been involved in various projects funded by the US Department of Energy and Advanced Research Projects Agency-Energy (ARPA-E) on bioreactors and Very High Temperature Reactor. In the PIRE project, he has been conducting research on drilling fluids.

Postdoctoral Fellow

Dinesh K. Kalaga

PhD Students

Six PhD students have been recruited to the PIRE project in year 1. One new PhD student (Artur Zych from Mechanical Engineering) and five existing PhD students (Manizheh Ansari, Fang Liu, Fanny Thomas, and Shaghayegh Darjani, from Chemical Engineering, and Geng Liu from Mechanical Engineering) have been conducting experimental, theoretical or numerical simulation research in different Research Thrusts. Recently, Yu Han from Chemical Engineering also joined the PIRE project. All of them are outstanding students and have received graduate fellowships with tuition waivers for up to five years from City College. Many of these PhD students have been engaged in similar research until this PIRE project was launched and they are expected to complete their PhD programs in Year 2 or 3 of this project.

PhD Students

Manizheh Ansari
PhD Student
Chemical Engineering

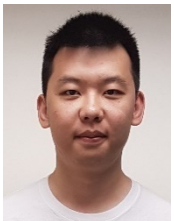
Shaghayegh Darjani
PhD Student
Chemical Engineering

Fanny Thomas
PhD Student
Chemical Engineering

Geng Liu
PhD Student
Mechanical Engineering

Fang Liu
PhD Student
Chemical Engineering

Artur Zych
PhD Student
Mechanical Engineering



Yu Han
PhD Student
Chemical Engineering

Master's Students

Two Master's students, James Barkas from Mechanical Engineering and Yamile Patino Vargas from Computer Science have been recruited in early 2018 to develop a PIRE database and website.

Master Students Year 2018

James Barkas
Master Student
Mechanical Engineering

Yamile Patino Vargas
Master Student
Computer Science

Project Coordinator and Internal Advisor

A project coordinator, Anna Volovik, was recruited from CUNY's John Jay College in October, 2017, and John Tsapogas of Research Foundation of CUNY was appointed as an internal advisor.

PIRE Project Coordinator: Anna Volovik **Internal Advisor**: Dr. John Tsapogas

PIRE Advisory Board

The PIRE project has an Advisory Board consisting of four academic members, Dr. Morton Denn (Albert Einstein Professor of Science and Engineering Emeritus, Levich Institute, and member of National Academy of Engineering), Dr. Dan McCloskey (CUNY's Interim Associate Vice Chancellor and University Vice Provost for Research), Dr. Lamia Goual (Associate Professor of Petroleum Engineering at the University of Wyoming), and Dr. Francisco Vargas (Louis Owen Assistant Professor of Chemical and Biomolecular Engineering at Rice University), and two industrial members, Dr. Oliver Mullins (Schlumberger Fellow and member of National Academy of Engineering), and Dr. Harald Kallevic (Equinor).

From left to right: Drs. M. Denn, D. McCloskey, L. Goual, and F. Vargas, O. Mullins and H. Kallevic

External Evaluator

An External Evaluator of this PIRE project is Dr. Denis Gray of North Carolina State University who has many years of experience in evaluating NSF programs of this scale.

International Collaborators

Our research collaborators include some of the most respected international researchers in the field from Norway, France and Germany. Norwegian collaborators include Drs. H. Linga, B. Lund, R. Larsen, and M. Fossen from Norwegian Foundation for Scientific & Industrial Research (SINTEF), Drs. Ole Jørgen Nydal and S. Sangesland from Norwegian University of Science and Technology (NTNU), and Drs. A. Jensen and A. Carlson from University of Oslo (UIO).

Norway

In France, our collaborators include Drs. O. Masbernat and M. Abbas from National Polytechnique Institute of Toulouse (INP-ENSIACET), Drs. L. Fournaison and A. Delahaye from National Research Institute of Science and Technology (IRSTEA), Dr. D. Dalmazzone from École Nationale Supérieure (ENSTA ParisTech), and Dr. A. Simon from Laboratoire de Chimie et Physique Quantiques (LCPQ).

France

German collaborators are Dr. M. Krause from Karlsruhe Institute of Technology (KIT), Dr. P.. Neumann from University of Hamburg (UH), Dr. G. Deerberg from Ruhr-Universität Bochum (RUB)/Fraunhofer UMSICHT, Drs. S. Gschwander and P. Schossig from Fraunhofer ISE, and Dr. U. Scheler from Leibniz Institut Dresden (IPF).

Germany

PROJECT GOALS

This PIRE Project has three major goals concerning research, education and international partnerships:

1. To advance knowledge and make transformative scientific discoveries to improve energy and process efficiency in industrial systems on a global scale.
2. To accelerate education and training of students and postdocs by providing unique opportunities in international research
3. To build strong international partnerships by sharing resources and research infrastructure within and across institutions

In Year 1, we have addressed all three goals by setting up four Research Thrusts and a Modeling and Simulation group, all of which involve researchers from CCNY and European institutions as listed below.

Research Thrust 1: Asphaltene Adsorption, Aggregation, and Interfacial Effects
CCNY: Pauchard, Banerjee, Messinger, Koplik, Lee, Liu, Darjani; SINTEF: Fossen, Larsen, INP-LGC: Masbernat, LCPQ: Simon; IPF: Scheler

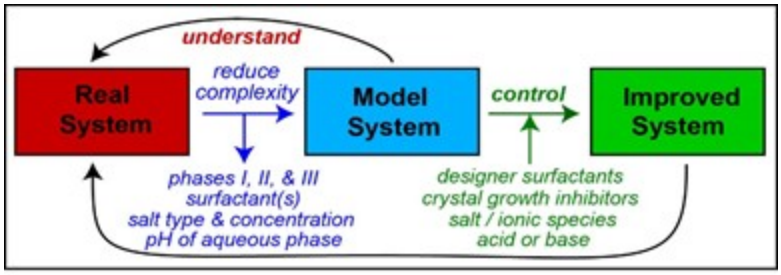
Research Thrust 2: Formation and Control of Gas Hydrate Slurries
CCNY: Morris, Pauchard, Kawaji, Banerjee, Messinger, Lee, Thomas; IRSTEA: Fournaison, Delahaye; ENSTA ParisTech: Dalmazzone; RUB/Fraunhofer UMSICHT: Deerberg, Janicki; SINTEF: Fossen, Larsen

Research Thrust 3: Drilling Fluids and Mechanisms of Particle Sedimentation
CCNY: Banerjee, Kawaji, Morris, Kalaga, Ansari; SINTEF: Linga, Lund, Larsen, Fossen; NTNU: Nydal, Sangesland, Skalle; UIO: Jensen, Carlson; INP-LGC: Masbernat, Abbas

Research Thrust 4: Phase-Change-Material Nanoemulsions for Energy Transport and Storage
CCNY: Kawaji, Messinger, Zych, Kalaga; Fraunhofer ISE: Gschwander, Schossig; IRSTEA: Delahaye, Fournaison; ENSTA ParisTech: Dalmazzone; INP-LGC: Masbernat; IPF: Scheler

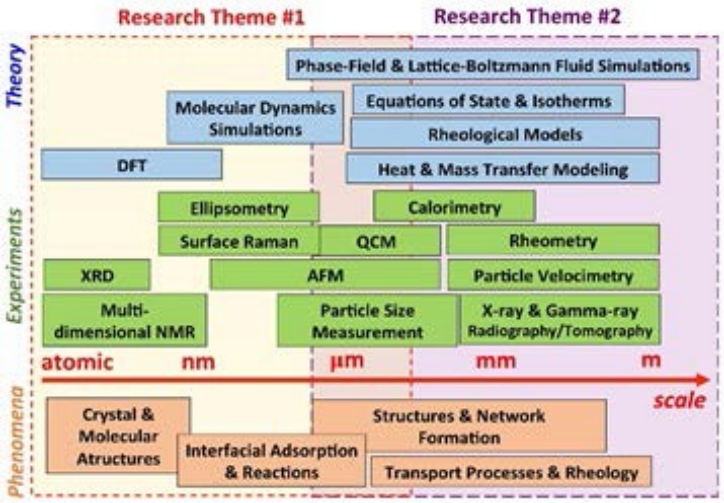
Modeling and Simulation
CCNY: Lee, Koplik, Banerjee, Liu, Darjani; KIT: Krause; U. Hamburg: Neumann; LCPQ: Simon

A unifying approach adopted by all Research Thrusts is to identify a model fluid or system with reduced complexity compared to the actual complex fluid. The model system for each Thrust should capture the relevant physics and chemistry and would then be studied in detail using the advanced research tools available at CCNY and collaborating institutions in order to yield improved multi-scale understanding of the original system. In addition, efforts will be made to identify the actions that can be practically and economically realized to control the formation of network structures, such as the addition of surfactants, crystal growth inhibitors, and salt or ionic species.



Unifying strategy for studying the proposed complicated, industrially relevant engineering systems

In Year 1, some of the cutting-edge experimental and theoretical techniques available at CCNY and collaborating institutions have been identified and utilized to probe physicochemical phenomena up from the atomic length scale to macroscale as shown below.



Advanced Research Tools available for Different Length Scales

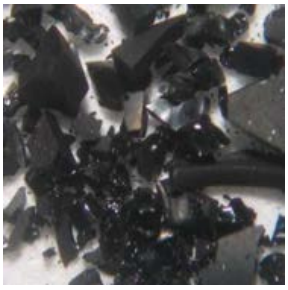
Our multi-national research collaborators possess proven track records in the development and application of many of these methods: e.g., multi-dimensional, pulsed-field gradient (PFG), and Rheo-NMR (Messinger and Scheler); X-ray and gamma-ray techniques (Kawaji, Banerjee and Jensen); phase change properties (Kawaji, Gschwander, Schossig, Fournaison and Delahaye); Planar Laser Induced Fluorescence, Tomographic PIV, Micro Raman Spectroscopy and DSC microscopy (Masbernat); lattice-Boltzmann simulations (Lee, Krause, Neumann, Banerjee, and Morris); Stokesian dynamics, rheometry, and flow modeling (Morris); pendant droplet and QCM (Pauchard); DFT (Aude); and MD (Koplik).

At the First Annual Review Meeting held at City College of New York on June 18-20, active discussions were held to promote sharing of these resources available at different institutions for each Research Thrust.

RESEARCH ACTIVITIES

In this section, the research activities from each Research Thrust are summarized.

Research Thrust 1: Asphaltenes (Thrust Leader: Dr. Robert Messinger)



Research on asphaltene adsorption, aggregation, and interfacial effects is conducted actively by CCNY researchers and international collaborators including Drs. Sanjoy Banerjee, Joel Koplik, Robert Messinger and Dr. Vincent Pauchard at CCNY, Drs. Aude Simon at LCPQ and Olivier Masbernat at INP-LGC in Toulouse, France, and Drs. Martin Fossen and Dr. Roar Larsen at SINTEF, Norway and Dr. Ulrich Scheler at IPF in Dresden, Germany. Asphaltenes are poly-disperse mixture of peripheral alkyl chains with different length, different heteroatoms with polar functionality in the PAH core, and have an average molecular weight of ~ 750 g/mol with a range from 400 to 1500 g/mol, are insoluble in alkanes but soluble in aromatic solvent, and the most polarizable and surface active component of the crude oil.

Experimental and theoretical investigations have been conducted by two PhD students in Chemical Engineering Department at CCNY, Shaghayegh Darjani and Fang Liu. Shaghayegh is studying the fluid to solid phase transition of asphaltenes laden interface. She is proposing a novel approach for driving the equation of state for a two-dimensional lattice gases. The relationship between surface coverage and excluded area is first extracted from random sequential adsorption. Then the adsorption isotherm and equation of state are obtained based on the kinetic argument and Gibbs adsorption isotherm. Her approach helps to understand better the adsorption of asphaltenes on the oil/water interface and explain some experimental observations like the appearance of wrinkles on the droplet covered by asphaltenes at high surface coverage. She has started using

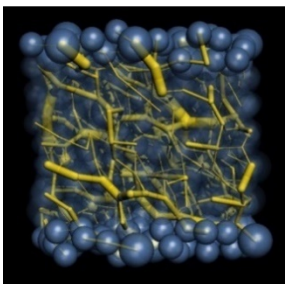
Self-Consistent-Charge Density-Functional-Tight-Binding method to extract the observables like molecular area, Gibbs free energy of adsorption and effective potential of interaction to provide the parameters for less refined models. Fang Liu is developing a methodology to predict asphaltenes adsorption behaviors and their effects, which are of great theoretical interest in upstream engineering for the oil industry. Fang is working closely with our partners at Multiphase Flow Assurance Centre (FACE) of SINTEF in Norway. Her research involves the study of asphaltenes interfacial behaviors at oil-water interfaces and the investigation of how asphaltenes precipitate onto the hydrophilic solid surfaces, and the mixture effects of asphaltenes on dilatational rheology behavior of asphaltenes-laden interface. Her work includes the development of the numerical simulations with non-convex optimization algorithms for adsorption behavior of asphaltenes mixture and the experimental study of asphaltenes adsorption on solid surfaces using quartz crystal microbalance with dissipation (QCM-D) technique. She is presently doing a summer internship at Materials, Corrosion and Flow Assurance group with ExxonMobil Upstream Research Company and is working on the investigation of asphaltenes deposition using QCM-D. In the future, NMR measurements applied to asphaltenes research will be conducted by Dr. Robert Messinger's group.

On March 15, 2018, both Shaghayegh Darjani and Fang Liu presented their research work on asphaltenes at the Mini-Workshop attended remotely by collaborators from France and Norway. On June 11, 2018, a Research Thrust meeting was held with European collaborators joining remotely by BlueJeans.

At the Annual Review meeting on June 18-20, 2018 attended by more than 40 researchers in person or by a web-meeting tool, BlueJeans, Fang Liu made a presentation entitled "Studies of Asphaltene Deposition onto Hydrophilic Surfaces Using Quartz Crystal Microbalance with Dissipation". From her work on asphaltene adsorption on the oil-water interface, Shaghayegh Darjani described DFTB and lattice gas absorption simulations, as well as dilatational rheology and expansion-contraction experiments. Dr. Martin Fossen of SINTEF gave a presentation entitled "Asphaltene Fractionation" as well. Active Q&A followed each presentation and the participants gained a better understanding of the fundamental scientific issues involved in the asphaltenes-related research in this PIRE project.

Since Dr. Vincent Pauchard left CCNY in January, 2018, Dr. Robert Messinger has been appointed as the Thrust leader for this Asphaltenes thrust, while Dr. Vincent Pauchard has continued to participate in the PIRE project as a guest researcher of the CUNY Energy Institute.

Research Thrust 2: Gas Hydrates (Thrust Leader: Dr. Jeffrey Morris)



Research to date at CCNY in Thrust 2, Hydrates, has focused on developing interfacial numerical tools that have been under development to apply to the problem of clathrate hydrate formation at interfaces as occurs in emulsions, the influence of flow processes on these, and how the hydrate affects the mixture flow properties. Fanny Thomas, a Ph.D. student advised by Dr. Morris and working collaboratively with Drs. Joel Koplik and Taehun Lee, has worked to develop a three-phase (solid hydrate with hydrocarbon and aqueous liquid) solver based on a diffuse interface model coupled to a lattice-Boltzmann solver. This will be developed in combination with experiments now started in collaboration with the laboratory of Dr. Didier Dalmazzone of ENSTA ParisTech, where Ms. Thomas will begin interning in September 2018, and will have involvement with the team at the laboratory IRSTEA (Drs. Laurence Fournaison and Anthony Delahaye) as well. The goal of the initial experiments is to establish the contact angle of cyclopentane hydrate with the CP-containing organic and aqueous phase, without and with surfactants. In a related effort, in which we are now involving Dr. Andreas Carlson of Univ. of Oslo, Dr. Joel Koplik has guided molecular dynamics to explore the microscopic physics of the contact line motion. Finally, work with Dr. Vincent Pauchard to model existing rheology data for CP hydrate forming emulsions has been undertaken by the Morris group. The researchers at LGC Toulouse (Drs. Olivier Masbernat and Sebastien Teychené) are also participating in this Research Thrust.

On March 15, 2018, a Mini-Workshop was held and F. Thomas gave a presentation entitled “Contact Line Dynamics and Capillary Forces in the Diffuse Interface Theory”. Notable comments and suggestions from the participants were that the relation of the numerical method to the hydrates problems needs to be made more explicit. Thus, a direct experimental study will be conducted by Ms. Thomas with hydrate-forming materials, beginning in summer 2018, to facilitate this effort. At the Research Thrust Meeting on June 5, 2018, the following presentations were given: J. Morris - “PIRE – Hydrates Thrust”; L. Fournaison - “Hydrate activities at IRSTEA”; Dr. Georg Janicki - “Hydrates research at RUR Bochum/Fraunhofer”. Notable comments and suggestions from participants were that the key issues which can be studied appear to be related to the influence of hydrates on rheology, as well as interfacial effects. Another key issue at the time of this meeting was on the development of a joint proposal by the French team members, and this was briefly discussed with input offline from the meeting provided by the CCNY team to more clearly establish links between the French ANR project with the CCNY PIRE studies. At the Annual Review meeting on June 18, 2018, a total of four presentations were given by CCNY researchers as well as French and Norwegian collaborators: J. Morris - “Hydrates at CCNY”; F. Thomas - “Contact Line Dynamics and Capillary forces in the Diffuse Interface Theory”; D. Dalmazzone - “Hydrates studies at ENSTA ParisTech” and Harald Linga - “Hydrates priorities at SINTEF”. Notable comments and suggestions from participants were that rheology and flow behavior provide an obvious place where all players have overlapping interest. Interfacial phenomena and the molecular environment need to be explored to obtain a scientific basis for the observed behavior, and molecular dynamics specific to the hydrate-forming system is an approach which all team members feel has relevance to pursue.

Research Thrust: Drilling Fluids (Thrust Leader: Dr. Sanjoy Banerjee)

In close collaboration with SINTEF researchers in Norway, the CCNY researchers (Drs. S. Banerjee, M. Kawaji, V. Pauchard, R. Messinger and D. Kalaga and a PhD student, M. Ansari) have been conducting experimental research on drilling fluids to better understand their behavior and improve their performance in the oil fields. The drilling fluids are used in oil fields to maintain safe and efficient drilling operations, and manage pressure in the wellbore to prevent water from seeping in from the surroundings. The oil-based drilling fluids also aid in transporting cuttings to the surface, cooling and lubricating the drill bit and drill string, and maintaining wellbore stability. They are non-Newtonian fluids composed of base oil, water, weighting agents, stabilizing agents, organophilic clays and other additives. Since the weighting agents (e.g. barite) are particulates that maintain the density of the drilling fluid, their settling ("aka sag") may result in loss of pressure control, uncontrolled flow of fluids from or into the formation and wellbore instabilities. The mechanism of sedimentation of barite particles as well as the rheological characteristics of drilling fluids are to be investigated in detail in this Research Thrust. Contacts have been made with the Norwegian supplier of commercial drilling fluids, MI Swaco, to obtain samples of the drilling fluids for testing at CCNY. After discussions with SINTEF researchers, Drs. Bjorner Lund and Harald Linga of SINTEF, and Richard Gyland of MI Swaco, individual components needed to prepare drilling fluids would be obtained and used to synthesize a model fluid with less complexity for testing and characterization purposes.

A postdoctoral researcher at CCNY, Dr. Dinesh Kalaga and a PhD student, Manizheh Ansari, have performed preliminary X-ray and Gamma densitometry measurements to standardize the experimental techniques in order to determine the rate of settling of Barite particles in the drilling fluid. A vertically traversing platform has been constructed to make gamma densitometry measurements on a drilling fluid sample in a 10 cm diameter tube at six axial locations. Several micro X-ray computed tomography (CT) equipment and facilities have been identified that would enable density distribution measurements in drilling fluid samples over a long duration. In parallel, Dr. Kalaga has been developing a pressure drop (using pressure transducers) and in-situ weight measurement methods (using a load cell) for Barite particle sedimentation measurements. Apart from the sedimentation measurements, Manizheh Ansari and Dr. Kalaga have also performed rheological measurements

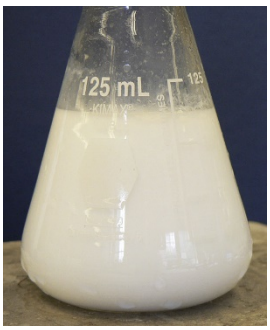
to understand the rheological behavior of the drilling fluid by varying shear rates (0.01-1000 1/s), angular frequency, oscillation displacement and temperature from 0 to 60 °C. Viscosity of the drilling fluid has been found to decrease with increasing temperature and shear rate confirming the shear thinning behavior of the fluid. M. Ansari is studying the link between the particle carrying capacity of the drilling fluids and their rheological properties and microstructure. Thus, she has been studying the impact of shear and mixing as well as individual components in the drilling fluids on the resulting fluid rheology. Since drilling fluids are normally designed with a finite yield stress, depending on the period of standstill, sufficiently small particles are suspended indefinitely. In the future, NMR spectroscopy will be utilized to study the importance of molecular interactions between the stabilizing agents and weighting agents.

At the mini-Workshop held on March 15, 2018, M. Ansari and D. Kalaga made a presentation entitled Drilling Fluids and Mechanisms of Particle Sedimentation". During the Research Thrust meeting on June 4, 2018, Mr. Richard Gyland of MI Swaco gave three presentations entitled "Oil based fluids – General Barite sag Micronized technology", "Oil based fluids Barite sag" and "Oil based fluids Micronized technology". Also, Dr. Harald Linga of SINTEF gave a presentation entitled "Autoviscosity - SINTEF R&D drilling fluid competence applied to a selected ongoing industry project". Mr. Gyland's presentations were informative and provided good background information for the drilling fluids research.

At the Annual Review meeting, Masahiro Kawaji briefly described the presentations that Mr. Gyland of MI Swaco had made at the Trust meeting, Dr. Harald Linga gave a presentation entitled "Drilling fluids – Recent and future research topics addressed at SINTEF, and M. Ansari and D. Kalaga presented the results of preliminary rheological measurements and particle sedimentation experiments.

Notable comments from participants were that testing model drilling fluids with less complexity and reduced number of components should lead to a better understanding of the effect of each component on rheological and particle sedimentation characteristics in drilling fluids.

Research Thrust 4: PCM Nanoemulsions (Thrust Leader: Dr. Masahiro Kawaji)



A new PhD student, Artur Zych, recruited in October, 2017, and a postdoctoral researcher, Dr. Dinesh Kalaga, recruited in March, 2018, have conducted research in the PCM Nanoemulsions Thrust. They first performed a literature survey covering our own publications, those of our collaborators at Fraunhofer ISE, and others. They studied different methods for synthesizing stable PCM Nanoemulsions, measuring rheological and phase change properties and heat transfer characteristics (heat capacity, latent heat of fusion, supercooling, and heat transfer coefficient), determining velocity characteristics and the effects of phase change. In addition, the concentration of PCM and type and concentration of surfactants were identified to be important parameters strongly affecting the energy storage capacity and viscosity.

As a first step, two different phase change materials, octadecane and paraffin wax with a melting point (m.p.) of 58 ^{o}C, have been used to synthesize PCM nanoemulsions using a Phase Inversion Temperature method. A Silverson homogenizer with a maximum speed of 10,000 rpm was purchased and used to produce droplets of less than one micron in mean diameter. Nonionic surfactants used were Span 60 and Tween 80 at varying concentrations to test the stability of the nanoemulsions synthesized. A dispersion analyzer (Lumisizer by L.U.M.) available in our laboratory has been checked for measurements of particle size distributions, creaming, agglomeration, flocculation, droplet coalescence, emulsification, dispersibility, shelf-life, and stability based on instantaneous detection of the space- and time-resolved extinction of the transmitted light across the entire length of a nanoemulsion sample. A variable-temperature rheometer (TA Instruments ARES-G2) available in our laboratory has also been checked for viscosity measurements.

Artur Zych attended a Rheology Workshop organized by Dr. Stefan Gschwander at Fraunhofer ISE in Freiburg, Germany, on March 6 and 7, 2018. Artur spent two more days at Fraunhofer Institute to discuss his research project with Dr. Gschwander. On March 27, 2018, Masahiro Kawaji visited Fraunhofer ISE, met with Dr. Gschwander and his colleagues, visited well-equipped nanoemulsion-related laboratories, and discussed future collaborations. On May 21-23, Masahiro Kawaji attended the PCM 2018 Conference in Orford, QC, Canada, and presented a paper entitled "Phase-Change-Material Nanoemulsions for Energy Transport and Storage". He again met with Drs. Gschwander and Biedenbach there and discussed plans for a future PhD student internship: Artur Zych to spend his 6-month internship in Germany at both Fraunhofer Institute ISE in Freiburg and Leibniz Institute in Dresden, Germany.

At the First Mini-Workshop on March 15, Artur Zych made a presentation entitled "Review of Phase-Change-Material Nanoemulsions for Energy Transport and Storage". Dr. Gschwander commented on the need to avoid any evaporation of water during viscosity measurements at high temperatures. At the Research Thrust Meeting on June 4, the following presentations were given: Michael Biedenbach – "Characterization of an n-Octadecane PCS in a 0.5 m^3 Storage Tank Test Facility"; Artur Zych – "Phase-Change-Material Nanoemulsions for Energy Transport and Storage"; Masahiro Kawaji – "Review of Phase-Change-Material Nanoemulsions Research" and "Modeling of a PCM Nanoemulsion" and Ulrich Scheler – "Stability and molecular mobility for phase-change materials". At the First Annual Review Meeting on June 18-20, the following presentations were given: Michael Biedenbach – "Heat Storage Capacity Characterization and Scale-up of Phase Change Slurries"; Artur Zych – "Progress on Phase-Change-Material Nanoemulsions Research for Energy Transport and Storage"; Masahiro Kawaji – "Review of Phase-Change-Material Nanoemulsions Research"; Ulrich Scheler – "Stability and Molecular Mobility for Phase-Change Materials" and Sebastian Gund – "Supercooling Effects in Phase Change Slurries".

Dr. Scheler's presentation on simultaneous Rheo-NMR measurements of velocity profile and rheological properties was particularly interesting and useful for our future work as his measurement apparatus can be operated at above and below the phase change temperature to investigate the effect of phase change on viscosity and heat transfer characteristics of PCM Nanoemulsions.

Modeling and Simulation (Thrust Leader: Dr. Taehun Lee)

In the Modeling and Simulation group, the participants include Drs. Joel Koplik, Taehun Lee, and Jeffrey Morris from CCNY, international collaborators, Drs. Aude Simon and Micheline Abbas from France, Drs. Mathias Krauss and Philipp Neumann from Germany, and Dr. Andreas Carlson from Norway. Three PhD students from CCNY, Geng Liu, Fanny Thomas, and Shaghayegh Darjani are involved in this research as well as two German PhD students, Marc Haussmann and Maximilian Gaedtke from KIT.

There are three major modeling approaches employed in the Modeling & Simulation thrust. In the continuum approach, the lattice Boltzmann method (LBM) is used, which is a minimal kinetic approach that recovers the near incompressible Navier-Stokes (NS) equations at low Mach number. As a kinetic method, LBM has a unique advantage over the conventional NS approach, namely, straightforward treatment of contact line slip and liquid wetting on moving inhomogeneous surfaces. This feature enables us to tackle some fundamental physical problems found in drilling fluids, gas hydrate slurries, and PCM nanoemulsions thrusts at substantially lower computational cost. Taehun Lee and Jeffrey Morris have developed an open-source LBM code suitable for the applications in wetting, emulsion stabilization, and capillary bridge. In year 1, this code was validated for the contact line motion of a liquid bridge and has been improved. One major outcome is the development of a novel "diffuse bounce back" scheme. The diffuse bounce back formula is obtained by applying a series of integration by part to the weak formulation of the lattice Boltzmann equation in multiple domains that consist of fluid and solid regions. It is designed to eliminate pressure fluctuation of the more popular "bounce back" scheme in LBM and to conserve mass in three-phase (liquid/liquid/particle) flows when

the particles are moving on a fixed background mesh. The researchers in the Modeling and Simulation group are in the process of carrying out standard benchmark tests and extending the diffuse bounce back scheme to particle sedimentation.

A systematic approach to the electrocoalescence of particle-laden drops has also just begun, involving Drs. Joel Koplik and Charles Maldarelli in the CCNY Chemical Engineering Department and a new graduate student Yu Han. In petroleum recovery, it is advantageous to remove the small emulsion drops of water, often coated with small particulates, that naturally contaminate crude oils and lead to corrosion, catalyst deactivation and other problems. The emulsions are generally charged, and an applied electric field can force the drops to coalesce and coarsen so that they settle out and may be easily separated. Theoretical approaches to the coalescence problem are difficult because of the contrast in time scales between slow viscous flow and rapid interfacial rearrangement, and complicated further by the presence of ions and solids. Initially, the slower parts of the process will be simulated by boundary integral methods, and subsequently the rapid interfacial rearrangements will be addressed by molecular dynamics simulations.

EDUCATIONAL GOALS

Over the five years of this project, a total of 7 PhD students will be supported and trained for four years each to conduct research, and three postdoctoral fellows for one to two years each, and two Master's students each year, one from engineering and the other from Computer Science, to work on the database and website development and maintenance. In addition, with financial support from the NSF-supported Louis Stokes Alliance for Minority Participation (LSAMP) program at City University of New York (CUNY), two undergraduate students from underrepresented groups are annually sent to collaborating institutions in Europe to experience summer internships.

Our major Educational goals were to:

- Mentor and train outstanding undergraduates, graduate students and postdocs
- Provide trainees with technical, cultural and collaborative skills to excel in the globalized scientific community
- Target underrepresented groups for recruitment of a diverse cadre of trainees
- Contribute to development of the US STEM workforce through internationalized research and technical training, curriculum development, and outreach.

In Year 1, we have been able to recruit six PhD students, one postdoctoral fellow, two Master's students and two undergraduate LSAMP students. The goals of mentoring and training of graduate students and postdocs are being carried out within the research thrusts and progress has been excellent as detailed elsewhere in this report. A primary focus of the remaining education and outreach goals is the internationalization of their research experience. Specific activities for students carried out for year 1 in support of this were short international research visits, attendance and participation in a Mini-Workshop and Annual Review Meeting along with our PIRE international research partners, and participation in our web-based Research Thrust meetings with the international partners. All of our PIRE graduate students participated in the Mini-Workshop, Annual Review Meeting and their Research Thrust web-based meetings.

Brief summaries of research and other activities conducted by the postdoctoral researcher and PIRE students are reported below.

Postdoctoral Fellow

Dr. Dinesh K. Kalaga - Drilling Fluids and Mechanisms of Particle Sedimentation

Dinesh Kalaga has performed preliminary X-ray and Gamma densitometry measurements to standardize the experimental techniques to determine the settling of Barite particles in a Drilling fluid sample obtained from MI-Swaco company. Three test sections with different thicknesses (2 mm, 5 mm, 10 mm) were fabricated to test the energy of the existing X-ray source and X-ray camera. Looking at the preliminary X-ray images he has learned that the camera should have high pixel density to measure the change in drilling fluid density with time. Currently, he is exploring several micro computed tomography (CT) facilities to get the measurements on drilling fluid samples. A platform that can traverse axially has been constructed to make the gamma densitometry measurements on 10 cm diameter drilling fluid sample at six axial locations. These gamma scans were made over seven days to see the change in the mud density with time. He is processing the data to measure the settling rate of the particles. He also looking at pressure drop (using pressure transducers) and in situ weighing methods (using load cell) to measure the settling rate. Apart from the sedimentation measurements, he has also performed rheological measurements to understand the rheological behavior of the drilling fluid by varying shear rates, angular frequency, oscillation displacement and temperatures. Viscosity of the fluid has been found to decrease with increases in the shear rate and temperature, confirming the shear thinning behavior of the fluid.

PhD Students

Manizheh Ansari - Drilling Fluids and Mechanisms of Particle Sedimentation

Manizheh Ansari, a PhD student in Chemical Engineering at City College of New York, is jointly supervised by Drs. Sanjoy Banerjee, Masahiro Kawaji, and Robert Messinger. Manizheh is studying the mechanisms of particle sedimentation in drilling fluids. In order to maintain safe and efficient drilling operations, management of pressure in the wellbore to avoid gas-kick is important. Oil-based drilling fluids serve this task and also aid in transporting cuttings to the surface, cooling and lubricating the bit and drill string, maintaining wellbore stability, and preventing formation damage by creating a filter cake sealing the rock pores. They are non-Newtonian and have a complex formulation, composed of base oil, water, weighting agents, stabilizing agents, organophilic clays and other additives. Since weighting agents (e.g. barite) are particulates that maintain the density of the drilling fluid, their settling ("aka sag") may result in loss of pressure control, uncontrolled flow of fluids from or into the formation and wellbore instabilities. Barite setting is not only a static problem, but is also seen under flow. In this part of the project, she addresses challenges related to the particle sedimentation in oil base drilling fluids and she tries to link the particle carrying capacity of fluids to their rheological properties and microstructure. Thus, she studied the impact of shear and mixing as well as individual components in the drilling fluids on the resulting fluid rheology. A model drilling fluid is defined here, comprised of an oil-water emulsion, a weighting agent, and two stabilizing agents. The rheological measurements of the base emulsion and the emulsion with solid additives, particularly structuring agents such as clays or weighting agents, were collected under different temperature (from 0 to 60 °C) and shear rates (0.01-1000 1/s). Different regimes are observed: a Newtonian behavior at low shear rate and a non-Newtonian (shear thinning) behavior at higher shear rate, and the limiting shear rate value between the two regimes being dependent on temperature. Rheology and sedimentation rate has been explored in-operando with gamma densitometry; X-ray method will be used alternatively in future. Since drilling fluids are normally designed with a finite yield stress, depending on the period of standstill, sufficiently small particles are suspended indefinitely. Whereas under dynamic, settling rate increases with shear rate and mixing rate. Furthermore, NMR spectroscopy will be utilized to study the importance of molecular interactions between the stabilizing agents and weighting agents.

Geng Liu – Modeling and Simulation using Lattice-Boltzmann Method

Geng Liu, a PhD student in Mechanical Engineering at CCNY, is supervised by Dr. Taehun Lee. Geng is studying the simulation and geometry optimization of multiple phase flows with lattice Boltzmann method, and in particular these days the diffuse bounce back lattice Boltzmann approach for recovering the classic no slip boundary condition in diffuse geometry. His project builds on the previous mature two-phase flow simulations with lattice Boltzmann method in Dr. Taehun Lee's group. He now makes contributions to the PIRE project led by Dr. Masahiro Kawaji and works on modeling and simulation to support the thrusts of Drilling fluids, Nanoemulsions and Gas hydrates.

Geng began to pursue his PhD at City College in January 2015, and has been focusing on the study of sensitivity based multphase flow topology optimization with lattice Boltzmann method since he finished all coursework in 2017. In his study on optimization, he has found that diffuse geometry plays an important role in modeling the problems smoothly. Based on Dr. Lee's multiphase flow lattice Boltzmann phase field formulation, Geng developed a diffuse geometry version and tested that with a 2D wetting wall problem. After Geng joined the PIRE Project in 2017, while the project required more study on simulations, Geng's research also moved to the diffuse bounce back lattice Boltzmann equation. The bounce back condition is directly incorporated into the lattice Boltzmann equation in this approach. Geng tested this method with Fortran codes written by himself and the applications are implemented on the two workstations and the cluster Ludwig with 10 nodes in Dr. Lee's lab. Under PIRE Project, Geng is now seeking for collaboration with Dr. Mathias Krause's group in

Karlsruhe Institute of Technology, Germany. Geng worked with Mathias years ago and both of them were among the pioneers who developed the Adjoint Lattice Boltzmann Method.

Shaghayegh Darjani – Fluid-to-Solid Phase Transition of Asphaltenes-laden Interface

Shaghayegh Darjani is a PhD student in Chemical Engineering Department at CCNY jointly supervised by Drs. Sanjoy Banerjee, Joel Koplik and Vincent Pauchard. She is also working closely with Dr. Aude Simon at LCPQ. Shaghayegh is studying the fluid to solid phase transition of asphaltenes laden interface. She is proposing a novel approach for driving the equation of state for a two-dimensional lattice gases. The relationship between surface coverage and excluded area is first extracted from random sequential adsorption. Then the adsorption isotherm and equation of state are obtained based on the kinetic argument and Gibbs adsorption isotherm. Her approach helps to understand better the adsorption of asphaltenes on the oil/water interface and explain some experimental observations like the appearance of wrinkles on the droplet covered by asphaltenes at high surface coverage. She has started using Self-Consistent-Charge Density-Functional-Tight-Binding method to extract the observables like molecular area, Gibbs free energy of adsorption and effective potential of interaction to provide the parameters for less refined models.

Fang Liu, a PhD student in Chemical Engineering at City University of New York City College, is developing the methodology to predict asphaltenes adsorption behaviors and their effects, which is of great theoretical interest in upstream engineering for the oil industry. Fang is jointly supervised by Dr. Sanjoy Banerjee at City College and Dr. Vincent Pauchard and will be working closely with our partners at Multiphase Flow Assurance Centre (FACE) of SINTEF Norway. Her research involves the study of asphaltenes interfacial behaviors at oil-water interfaces and the investigation of how asphaltenes precipitate onto the hydrophilic solid surfaces. Fang started her residency at City College in mid-August (2013) and have published her work on the mixture effects of asphaltenes in dilatational rheology behavior of asphaltenes-laden interface in Langmuir. Her most recent work includes the development of the numerical simulations with non-convex optimization algorithms for adsorption behavior of asphaltenes mixture and the experimental study of asphaltenes adsorption on solid surfaces using quartz crystal microbalance with dissipation (QCM-D) technique. She is presently doing a summer internship at Materials, Corrosion and Flow Assurance group with ExxonMobil Upstream Research Company and is working on the investigation of asphaltenes deposition using QCM-D.

Artur Zych – Synthesis and Characterization of PCM Nanoemulsions

Artur Zych, a PhD student at City College of New York is supervised by Dr. Masahiro Kawaji and closely working with another graduate student James Barkas to study Phase Change Material (PCM) Nanoemulsions: how to create them in order to utilize their properties for effective heat storage and transport. He is conducting experiments in order to synthesize a stable nanoemulsion of PCMs by using two different techniques: low energy and high shear homogenization. Evaluating these techniques with different surfactants and diverse ratios of surfactant-to-paraffin to obtain a stable nanoemulsion for heat storage and transport. These experiments involve using a centrifuge to increase strength of gravity in order to quickly determine the stability and shelf-life of these nanoemulsions as well as finding the average diameter and size distribution which can have large influences on the flow and heat transfer characteristics. Artur Zych plans on studying the effect of these PCM nanoemulsions on fluid flow in a pipe and its consequence on heat transfer. Artur and James are currently supervising a high school student in creating these PCM nanoemulsions and exposing them to a higher level of research. Artur attended a Rheology Workshop organized by our collaborator, Dr. Stefan Gschwander, at Fraunhofer ISE in Freiburg, Germany, in March, 2018. Future measurements of particle size distributions in PCM Nanoemulsion samples at Fraunhofer ISE are planned.

Fanny Thomas – Wetting Phenomena in Gas Hydrates Slurries

Fanny Thomas is a PhD student in Chemical Engineering at City College of New York and has been studying the wetting phenomena which are believed to play a crucial role in the formation and control of gas hydrates slurries. In this project, the dynamics of capillary bridges and the motion of the three-phase contact line are studied within the framework of the diffuse interface theory. The key to understanding the dynamics of interfacial systems lies in an accurate description of the capillary forces governing the motion of the fluid and the solid elements. In this work, we combine the diffuse interface theory with a multiphase lattice Boltzmann algorithm to develop a description of the capillary forces in 2D binary interfacial systems on a continuum level. The method has been implemented for a pair system composed of a single bridge connecting two solid elements. We can identify the mechanisms governing the motion of the three-phase contact line and how the model handles the contact line singularity in comparison with the classic sharp-interface approach. We are now facing numerical challenges regarding moving boundaries and the tracking of the interface. Numerical results are validated by comparison with theoretical predictions at equilibrium. We have started the molecular dynamics simulations to get some physical insight on some of the parameters of the diffuse model. Experiments on the wetting properties of actual hydrate particles are expected to start end of July 2018. In December, 2017, she visited collaborators in Toulouse (INP) including Drs. Olivier Masbernat and Benjamin Lalanne. In June, 2018, she gave a talk entitled "Dynamics of capillary bridges and the three-phase contact line using a diffuse interface method" at the American Chemical Society's Colloid and Surface Science Symposium at Penn State. In early July, she visited ENSTA ParisTech and met with Dr. Didier Dalmazzone in preparation for the internship in his laboratory starting on September 1st, 2018.

Yu Han - Electrocoalescence of Particle-laden Drops

Yu Han is a PhD student in Chemical Engineering and has started working with Drs. Joel Koplik and Charles Maldarelli this summer on a systematic investigation of electrocoalescence of particle-laden water drops and use of an electric field to force the drops to coalesce for faster separation from crude oil.

Master's Students

One of the contributions of our PIRE to STEM workforce development is to provide talented masters students the opportunity to gain computer science related experience by participating in the development of our PIRE database and web applications. Two such masters students were supported for these tasks in our first year, CCNY Mechanical Engineering student James Barkas and CCNY Computer Science student, Yamile Vargas.

James Barkas, a Master's student in Mechanical Engineering at CCNY, has been involved in laboratory research on PCM Nanoemulsions for thermal energy storage, the development of the PIRE database, and has also provided logistical support for PIRE meetings, teleconferences and the Annual Review meeting in June 2018. James is working with Artur Zych on his doctoral research, developing PIT-based ("Phase Inversion Temperature") processes for producing paraffin-in-water PCM Nanoemulsions, as well as characterizing these emulsions in terms of their stability, viscosity, paraffin particle size distribution and effective heat capacity. The current focus is on developing paraffin-in-water emulsions that remain stable for months to years at a time across the anticipated operating temperature range of PCM Nanoemulsions for thermal storage applications (~25°C-60°C), selecting effective surfactants and co-surfactants, and identifying minimum surfactant concentrations to achieve the desired Nanoemulsion operating life. On-going work also includes assembling a heat transfer flow loop for measuring convective heat transfer coefficients and pressure losses of these Nanoemulsions.

Database development is being undertaken in collaboration with Jamila Patino Vargas. Work thus far has consisted of contacting individual PIRE participants, polling them about their data-handling and -sharing

needs, and collecting samples of data file formats in which they expect to generate as part of their PIRE research. PIRE researchers have also been asked to discuss and reach a consensus on what collaborations they will undertake, what data exchange needs they will have, and what the fate of the aggregated PIRE research data should be after the PIRE project is completed. Technical and logistical support for the PIRE has involved setting up, testing and performing trouble-shooting for AV equipment used in PIRE meetings including Research Thrust meetings and the Annual Review meeting, as well as moderating teleconferences between American and European collaborators.

Yamila Patino Vargas, a Master's student in Computer Science Department at CCNY has been developing a PIRE website since March, 2018. This website was opened to the public in May, 2018, and has links to the home pages and web sites of some of the PIRE faculty, students and collaborating researchers and their institutions.

https://pire.ccny.cuny.edu/

This PIRE website also has a useful feature to allow uploading and downloading of presentation files and documents which the participants in Thrust meetings and Annual Review Meeting can access, eliminating the need to send the files by e-mail. Additional features will be developed and incorporated into our website in the future.

NYC-LSAMP Undergraduate Students

The primary programmatic activity aimed at the goal of targeting underrepresented minority students is the international summer research internship for two undergraduate students from the CUNY Louis Stokes Alliances for Minority Participation (LSAMP) program. Students selected for this program spend two-months conducting research in our international partners research labs and give a presentation on their research and cultural activities upon their return. They also must provide written research summaries. For the summer of 2018 both students are in France; a CCNY Chemical Engineering student, Amy Chacon was placed at ENSTA-Paris and a CCNY Mechanical Engineering student, Michael Ramundo, was placed at IRSTEA in Paris.

Amy Chacon (CCNY Chemical Engineering)
Research Advisor: Dr. Didier Dalmazzone, École Nationale Supérieure de Techniques Avancées (ENSTA ParisTech)
Research Topic: Rheological Study of Gas Hydrate Formation for Drilling Fluid Applications

The oil industry continuously faces severe safety and economic threats, one of the largest problems is the formation of gas hydrates in drilling equipment. Depending on the thermodynamic conditions present while drilling, and the chemical and physical nature of drilling fluid formulations, (that are key in drilling processes) gas hydrates can form within drilling operations equipment. These hydrates can harm drilling operators and the problems can extend to severely damaging drilling equipment, resulting in economic loses. As a solution to these issues, the rheological properties (e.g. viscosity) of gas hydrates are studied. In conjunction to the rheology, the thermodynamic conditions, and phase behavior of gas hydrates are studied. In this report, the thermodynamics, phase behavior, and rheological profiles of carbon dioxide and methane hydrates are studied. The objective of this study will be to characterize gas hydrate formation in the simplest of scenarios (e.g in pure water) to build a foundation to characterize hydrates in more practical conditions, such as in drilling fluids. This will ultimately allow one to better understand when hydrates form (under what conditions) and how their formation can be minimized. To do this, a rheometer is used. The rheometer allows one to study the flow properties of gas hydrate formation in different kinds of fluids. Our goal is to reach a positive outcome from these experiments of reducing the amount of gas hydrates formed in drilling fluids.

Michael Ramundo (CCNY Mechanical Engineering)

Research Advisor: Dr. Laurence Fournaison, National Research Institute of Science & Technology for Environment & Agriculture (IRSTEA)
Research Topic: Clathrate Hydrate Formation Kinetics and Thermodynamic Cycles: Utilizing the Joule Thomson Effect to Form Hydrates Through High Pressure Shift Freezing

Clathrate hydrates, also known as gas hydrates, are an ice like solid crystalline compound that have gas atoms or molecules encaged in its crystal lattice. The water molecules encage the guest molecules by way of hydrogen bonds that are stabilized by van der Waal's forces. Gas hydrates are an ideal structure for multiple application since they are stable, and can efficiency contain gas molecules under STP. In the oil and gas industry, gas hydrates can form in transport pipes under high pressure and low temperatures causing flow stopping obstructions. Other than blocking fluid flow, they can become down flow projectiles causing pipe failures at elbows if the gas hydrate mass separates from the wall where it agglomerated. Natural gas hydrates can contain as much as 180 standard cubic feet of gas per cubic foot of solid natural gas hydrate. In order to utilize these materials for industrial applications an economical method of artificial production must be developed. Hydrates can form in a range of temperatures and pressures. This report will study the formation kinetics and thermodynamic cycle of the clathrate hydrates, 〖CO〗_2+H_2 O, while utilizing the Joule-Thomson effect for the process of high-pressure shift freezing. It will be tested if this method can produce hydrates and is economically viable for the industrial manufacture of these phase change material (PCM) slurries without the need for a scraped surface evaporator or mechanical mixing device to crystallize.

INTERNATIONAL COLLABORATION

Many opportunities were created to enable PIRE researchers to interact and collaborate with international collaborators through web-based Research Thrust meetings, Annual Review Meeting, and mutual visits as summarized below.

- A Mini-Workshop was held on March 15, 2018, covering all four Research Thrusts and Modeling & Simulation with more than ten international collaborators joining remotely via a web meeting tool, BlueJeans. All PhD students made presentations and discussed their work with participating researchers. Due to the time difference between New York and Europe, this Workshop was limited to 3 hours in the morning, 9 am – 12 pm in New York and 3 – 6 pm in Europe.

- Research Thrust meetings were held with international collaborators in all four Thrusts and Modeling in early June. Each meeting was two hours in duration and some European collaborators made presentations from their side.
  - June 4: Thrust 3 - Drilling Fluids
  - June 6: Thrust 4 - PCM Nanoemulsions
  - June 7: Modeling and Simulation
  - June 8: Thrust 2 - Gas Hydrates
  - June 11: Thrust 1 - Asphaltenes

The following mutual visits have been made by PIRE faculty, students, and collaborating researchers.

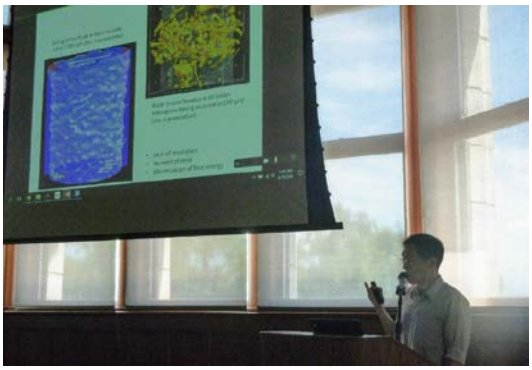
- Dr. Harald Linga attended the PIRE Opening Reception held at City College of New York on December 6, 2017, and met with PIRE faculty and students at CCNY.
- Dr. Taehun Lee visited and met with Drs. Olivier Masbernat and Micheline Abbas at the University of Toulouse (January 13 - 24, 2018), and was able to identify research topics for future collaboration in the PIRE project.
- Dr. Jeff Morris visited LGC Toulouse on February 18, 2018, and met with Drs. Olivier Masbernat, Sebastien Teychené, and Micheline Abbas. The possible experimental program to couple with CCNY simulations was the primary point of discussion.
- A PhD student, Artur Zych, attended a Rheology Workshop (March organized by our collaborator, Dr. Stefan Gschwander, at Fraunhofer ISE in Freiburg, Germany. Future measurements of particle size distributions in PCM Nanoemulsion samples at Fraunhofer ISE were discussed.
- From March 27 to April 6, Dr. Masahiro Kawaji visited French (IRSTEA and ENSTA-ParisTech), German (Fraunhofer ISE and RUB/Fraunhofer UMSICHT) and Norwegian (SINTEF and NTNU) collaborating institutions. He met with collaborating researchers (Drs. L. Fournaison, A. Delahaye, D. Dalmazzone, S. Gschwander, H. Linga, B. Lund, O.J. Nydal, S. Sangesland, and G. Janicki), briefed them on the PIRE project, visited their research facilities and discussed future collaborations and activities including the Thrust meetings and Annual Review Meeting planned in June.

- Dr. Ole Jørgen Nydal from NTNU visited CCNY on April 22, 2018, to see CCNY's research facilities.
- Fanny Thomas visited LGC Toulouse on March 5, 2018, and had discussions with Drs. Micheline Abbas, Olivier Masbernat and Sebastien Teychené, on interfacial numerical modeling, and appropriate experiments to be performed with emulsions, using microfluidic techniques of Teychené.
- On June 18-20, Drs. L. Fournaison, A. Delahaye (IRSTEA), D. Dalmazzone (ENSTA-ParisTech), H. Linga, Stian Fjermestad (SINTEF), A. Carlson and A. Jensen (NTNU), Max Gaedtke, Marc Haussmann, and Sebastian Gund (KIT) participated in the First Annual Review Meeting at CCNY and visited CCNY's research laboratories. Stian Fjermestad (SINTEF), a PhD student conducting research at SINTEF will spend one year as an internship student at CCNY in 2019.
- On July 2, 2018, Fanny Thomas visited Dr. Didier Dalmazzone at ENSTA ParisTech, and toured his laboratory, and established the priorities for an internship starting in September, 2018.
- On July 17-19, 2018, Dr. Jeff Morris visited LGC Toulouse. It was a combined visit associated with a separate program (FERMAT Foundation research chair) during which discussions with Dr. Masbernat's team related to experiments in the funded ANR program were the primary focus.

ANNUAL REVIEW MEETING

The First Annual Review Meeting (ARM) was held at City College on June 18-20, 2018. A total of ten collaborating international researchers attended this meeting in person, and additional 12 researchers joined via BlueJeans. On June 17, a casual reception was held at a local restaurant to welcome some of the European collaborators. The agenda for the meeting on June 18-20 is shown in Appendix 1. In each morning session,

presentations were made by the PIRE faculty, students and international collaborators in person or via BlueJeans. In the afternoon, more detailed discussions were held in separate Thrust meetings, and lab tours were given including CUNY's advanced Science Research Center (ASRC) located on the CCNY campus.




During the Annual Review Meeting, plans for PhD student internships in Year 2 were discussed. Mr. Stian Fjermestad, a PhD student from the University of Bergen and SINTEF in Norway, plans to spend one year at CCNY to work on a PIRE project.

On the second day of the ARM, an Advisory Board meeting was held with an agenda shown in Appendix 2. All Board members except for Dr. H. Kallevic from Norway were able to attend the meeting in person (Drs. M. Denn and D. McCloskey) or via BlueJeans (Drs. Goual, Vargas and Mullins). After the introduction of all PIRE faculty and students, and representatives of international collaborators (Drs. L. Fournaison and H. Linga), an overview of the PIRE project and progress made in Year 1 were given by the PIRE Project Director (M. Kawaji), followed by Thrust leaders (M. Kawaji, T. Lee, R. Messinger and J. Morris) and International Team Coordinators (L. Fournaison and H. Linga) offering the team leadership's viewpoints and concepts of synergy. The Advisory Board also met with all the PIRE students and postdoctoral researcher as outlined in the meeting agenda (Appendix 2).

OUTREACH ACTIVITIES

In Year 1, a summer internship for one high school student from Ossining High School in northern Westchester county in New York was arranged after meeting with Ossining High School's science teacher (Angelo Piccirillo) and a student (Nikita Subramanian) on April 20. Nikita is currently spending her summer internship in the PCM Nanoemulsions laboratory and working on a PCM Nanoemulsions research project supervised by Artur Zych and James Barkas. She is learning how to synthesize PCM Nanoemulsions and measure particle size distributions and supercooling effects using Lumisizer and Differential Scanning Calorimeter, respectively. She will return next summer to continue her research work on PCM Nanoemulsions. Next summer, we intend to invite and engage a few additional high school students from Ossining High School as well as local high schools in summer internships in PIRE-related projects.

On July 15-22, 2018, four graduate students, Andreas Reischl, Matthäus Lenz, David Schweinzer and Michael Puttinger from the Technical University-Graz in Austria, stayed at CCNY and participated in the LSAMP-sponsored Two-week Seminar Course on "Science and Society – In the Future". Our PhD students in the PIRE project presented and discussed their research work at a special meeting on July 18, and conducted a lab tour for them.

PIRE-RELATED EVENTS

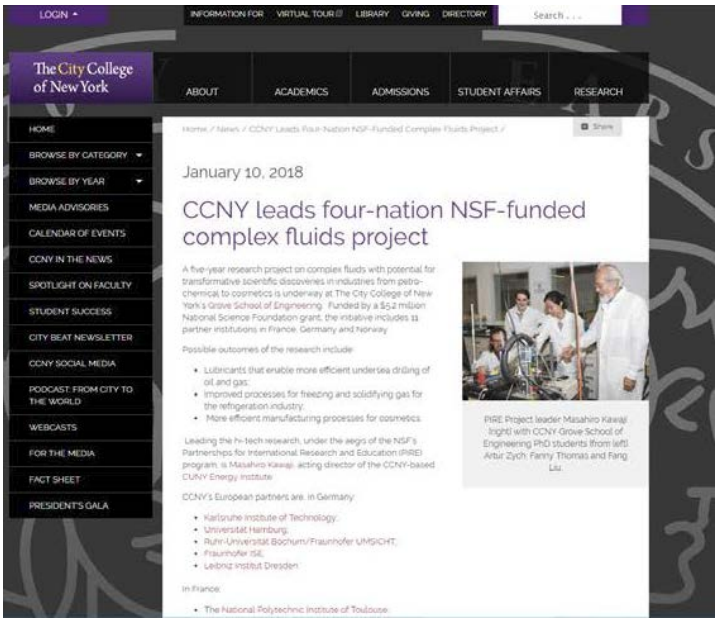
The **first CUNY International Research and Education Forum** was held at the CUNY Graduate Center on November 8, 2017. The PIRE PI, Dr. Masahiro Kawaji, presented a talk on the PIRE project in the session on CUNY's International Research Projects and explained the work involved in preparing an application for NSF's PIRE Program. At this forum, representatives of six foreign funding agencies including Dr. Berit Johne of the Research Council of Norway, gave panel presentations on their programs for international research collaboration. On the following day, Dr. Berit Johne visited CCNY and met with some of the PIRE Faculty and students, and also toured the research facilities used in the PIRE project.

Opening Reception

After launching of the PIRE project, an Opening Reception was held at CCNY on December 6, 2017, with all the PIRE faculty, PhD students and staff in attendance. The senior leadership of both CUNY (Dr. Vita Rabinowitz, Executive Vice Chancellor and University Provost, and Dr. Daniel McCloskey, Interim Associate Vice Chancellor for Research) and CCNY (Dr. Vincent Boudreau, President, and Dr. Mary E. Driscoll, Interim Provost and Senior Vice President of Academic Affairs) gave speeches promising support for this first PIRE project at CUNY. Dr. Harald Linga from Norway also attended this event as a representative of our European collaborators.

On January 10, 2018, CCNY published an on-line article concerning the launch of the PIRE project.

https://www.ccny.cuny.edu/news/ccny-leads-four-nation-nsf-funded-complex-fluids-project



PIRE Website

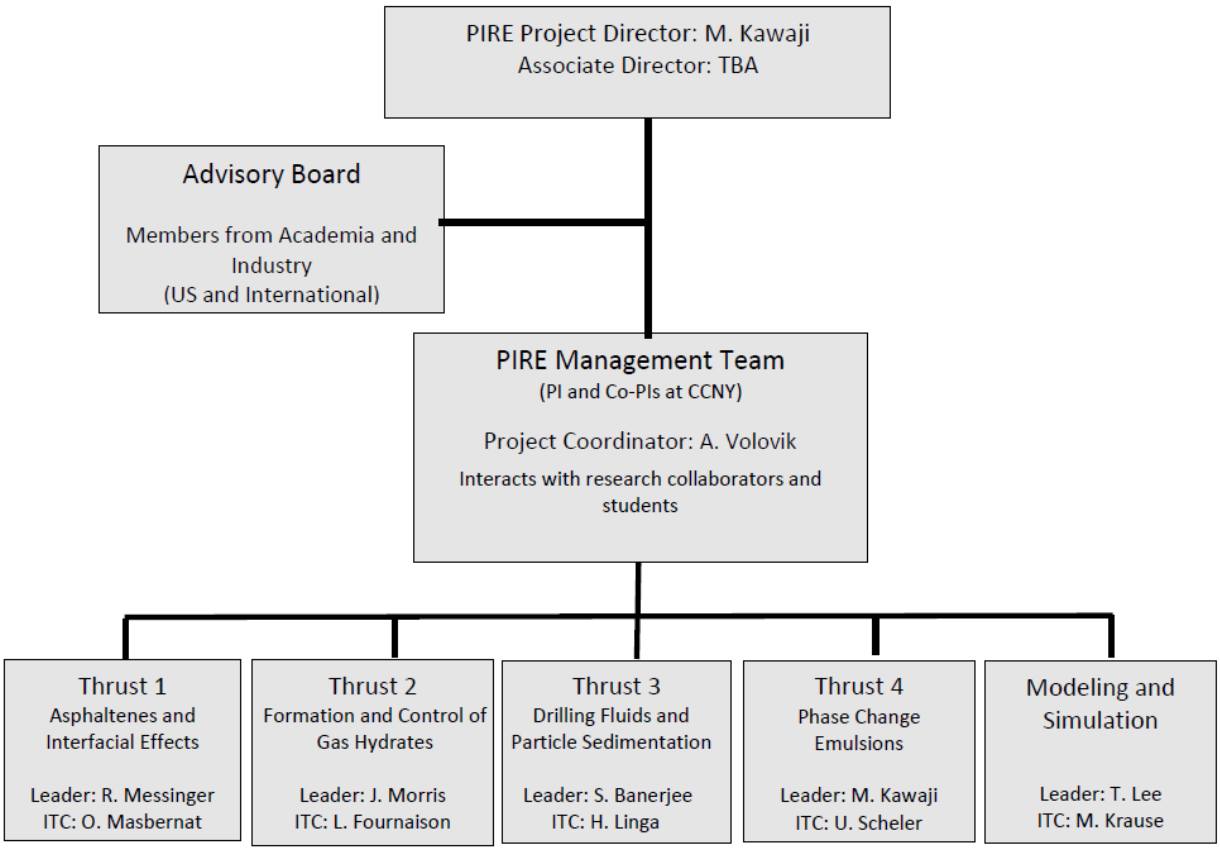
The PIRE project's website was developed by Yalemi Patino Vargas, a Computer Science Master's student at CCNY.

https://pire.ccny.cuny.edu/

This website was opened to the public in May, 2018, and has links to the researcher's home page and web sites of collaborating institutions. It also has a useful feature to allow uploading and downloading of presentation files and documents remotely by the participants in Thrust meetings and Annual Review Meeting, eliminating the need to send the files by e-mail. Additional features will be developed and incorporated into our website in the future.

PROJECT MANAGEMENT

The structure of the PIRE management is shown below. It has been revised from that originally proposed, but the main roles of the PIRE Project Director, Project Coordinator, PIRE Management Team, Advisory Board, and Research Thrust Leaders and International Technical coordinators (ITC's) have remained the same. Dr. Robert Messinger was appointed as the leader for Research Thrust 1 on Asphaltenes, replacing Dr. Vincent Pauchard who left City College in January, 2018, but is still participating in the PIRE project as a guest researcher of the CUNY Energy Institute.



PIRE Project Management Structure

In order to ensure the success of this PIRE project, monthly PIRE Management Team meetings have been held on October 16 and November 20, 2017, and February 9, March 14, April 19, May 16, June 6, and July 11, 2018. At each management meeting, meeting agendas are distributed and kept for filing.

On April 9-10, 2018, NSF organized a meeting for the PIRE Project PI's in Alexandria, VA. The Project PI (M. Kawaji) and Project Coordinator (A. Volovik) attended this meeting and received many constructive suggestions from the NSF staff and other PIs of the PIRE projects already in their 3rd and 5th years.

DISSEMINATION OF RESEARCH RESULTS

Some results from the work underway in this PIRE project have been published in journals and presented in conferences and seminars by CCNY's PIRE faculty and students as summarized below.

- Shaghayegh Darjani, Joel Koplik, and Vincent Pauchard, "Extracting the equation of state of lattice gases from random sequential adsorption simulations by means of the Gibbs adsorption isotherm," Physical Review E, 96, 052803 (2017). DOI: 10.1103/PhysRevE.96.052803.

- Masahiro Kawaji, "Phase-Change-Material Nanoemulsions for Energy Transport and Storage" Proc. Of the 12th IIR Conference on Phase Change Materials and Slurries for Refrigeration and Air Conditioning, Orford, Québec, Canada, May 21-23, 2018. DOI: 10.18462/iir.pcm.2018.0044

- Taehun Lee gave an Invited seminar: "Computational Study of Microparticle Effect on Self-propelled Jumping of Droplet," Department of Mechanical Engineering, Binghamton University, Oct. 25, 2017.

- Taehun Lee, “Interface Tracking, Surface Tension, Boundary Conditions and Discretization in Multi-Phase Lattice Boltzmann Method”, presented at the 27th International Conference on Discrete Simulation of Fluid Dynamics, June 25- 29, 2018, Worcester Polytechnic Institute, Worcester, MA.

- Lina Baroudi and Taehun Lee, “Lattice Boltzmann Simulation of Initial Spreading of Low-Viscosity Drops”, presented at the 27th International Conference on Discrete Simulation of Fluid Dynamics, June 25- 29, 2018, Worcester Polytechnic Institute, Worcester, MA.

- Jeffrey Morris - Nordic Rheology Conference, June 13-15, Trondheim, Norway.
    - Delivered a short course lecture entitled “Rheology: Basic concepts and measurement, with some physics for particulate systems” to 25 participants from Scandinavian companies and universities, combined with SINTEF and NTNU practical component.
    - Gave a Plenary address entitled “Extreme transitions of flow properties: hydrate jamming & discontinuous shear thickening”

- Fanny Thomas and Jeffrey F. Morris, “Contact Line Dynamics and Capillary forces in the Diffuse Interface Theory”, presented at the American Chemical Society’s Colloid and Surface Science Symposium, June 10-13, 2018, Penn State University, State College, Pennsylvania.

EXTERNAL EVALUATOR'S REPORT (Dr. Denis Gray)

The PIRE External Evaluator, Dr. Denis Gray, visited CCNY on June 5 and met with the PIRE faculty and students. After the introductions, Dr. Masahiro Kawaji presented an overview of the PIRE project. Dr. Gray then explained the evaluation methodology and criteria. Afterwards, a guided tour of the PIRE research facilities was conducted including the CUNY Advanced Science Research Center (ASRC).

On June 18-20, Dr. Gray attended some sessions in the Annual Review Meeting remotely and conducted an evaluation of the activities in Year 1 of this PIRE project. His draft report is attached as Appendix 3 which also includes a summary of a survey of the Annual Review Meeting among the participants. The abstract of a draft evaluation report is shown below.

Abstract of a draft Evaluation Report by Dr. Denis Gray

Consistent with its proposal PIRE at CCNY Multi-Scale, Multi-Phase Phenomena in Complex Fluids for the Energy Industries project will participate in an evaluation by an external evaluator. The focus of this evaluation during the early stages (years 1 and 2), will be on monitoring and formative evaluation efforts. This evaluation report (a draft attached in Appendix 3) focuses on the implementation of the project plan and feedback from the project's first annual meeting.

In order to facilitate the ongoing evaluation of the project a logic model (Appendix 3A) was developed which graphically displays what activities will lead to various project outputs (short term), outcomes (midterm) and impacts (long term). Program documents were used to assess the extent to which various implementation activities detailed in the logic model have been planned and/or implemented to achieve project outcomes and impacts. As detailed in the report the project PIs have made tremendous progress in standing up the project in all of the project domains including: Project Management, Knowledge Advancement, Education and Training, Recruitment of Underrepresented Students, Undergraduate/High School Research Experiences. Among these areas the recruitment of the first cohort of students, beginning international collaborations, and beginning international internships appear to be outstanding examples of the implementation effort.

Another area of success was the planning and implementation of the annual PIRE meeting held in June of 2018 that was attended by 44 individuals. A feedback survey about this event was conducted and achieved an enviable 82% response rate. Feedback was provided by both U.S. and non-U.S. attendees and in-person and virtual attendees. Ratings of the usefulness of the meeting sessions were uniformly high (averaging "very useful (4/5-point scale). Most suggestions for improvement focused on the thrust sessions and indicated these sessions should be given more agenda time and become more interactive in the future. Ratings for achieving various meeting objectives (become more familiar with project scope and goals; become more familiar with research performed and planned in various thrusts; meet and network with other participants; discuss opportunities to share resources and collaborate; identify institutions for international student placements) were also rated consistently high (average rating somewhere between agreed (4) and strongly agreed (5)). Only minor suggestions for improving PIRE, its research and future meetings were provided.

While work remains in a number of areas including education and training, underrepresented recruitment and high school experiences, based on my assessment the PIRE at CCNY has had a very productive and effective first year.

Appendix 1: Agenda of the First Annual Review Meeting

PIRE Project Annual Review Meeting Agenda

The City College of New York, CUNY

June 18th – 20th, 2018

Please Note: Sessions in purple color are open for remote participation via BlueJeans.

Day 1: Monday, June 18th			
New York Time	**European Time**	**Session**	**Location**
8:30	14:30	Continental Breakfast	350 Shepard Hall (3rd Fl.)
9:00	15:00	Opening Address and Introductions	350 Shepard Hall (3rd Fl.)
9:20	15:20	Overview of the PIRE Project	350 Shepard Hall (3rd Fl.)
9:45 – 11:00	15:45 – 17:00	Thrust 3: Drilling Fluids	350 Shepard Hall (3rd Fl.)
11:00 – 12:15	17:00 – 18:15	Thrust 1: Asphaltenes	350 Shepard Hall (3rd Fl.)
12:15 – 12:30	18:15 – 18:30	Welcoming Address by Vincent Boudreau, President of the CCNY	350 Shepard Hall (3rd Fl.)
12:30 – 2:00	18:30 – 20:00	Lunch	Faculty Dining Room
2:00 – 3:30	20:00 – 21:30	Lab Tours	Steinman Hall
3:30 – 5:00	21:30 – 23:00	Break-Out Meetings: Thrust 3: Drilling Fluids Thrust 1: Asphaltenes	 Energy Institute Conf. Room Dean's Office Conf. Room
Day 2: Tuesday, June 19th			
8:30	14:30	Continental Breakfast	350 Shepard Hall (3rd Fl.)
9:00 – 10:15	15:00 – 16:15	Thrust 2: Gas Hydrates	350 Shepard Hall (3rd Fl.)
10:15 – 11:30	16:15 – 17:30	Thrust 4: Nanoemulsions	350 Shepard Hall (3rd Fl.)
11:30 – 12:30	17:30 – 18:30	Modeling & Simulation Thrust	350 Shepard Hall (3rd Fl.)
12:30 – 2:00	18:30 – 20:00	Lunch	124 Steinman Hall (1st Fl.)
2:00 – 3:30	20:00 – 21:30	Break-Out Meetings: Thrust 4: Nanoemulsions Thrust 2: Gas Hydrates	 Energy Institute Conf. Room Dean's Office Conf. Room
3:30 – 5:00	21:30 – 23:00	Advisory Board Meeting	Energy Institute Conf. Room
6:00	00:00	Dinner for PIRE Faculty, European Collaborators & Advisory Board Members Dinner for the City College & European Students	Bryant Park Grill TBA
Day 3: Wednesday, June 20th			
New York Time	**European Time**	**Session**	**Location**
8:30	14:30	Continental Breakfast	350 Shepard Hall (3rd Fl.)
9:00 – 10:00	15:00 – 16:00	PIRE Website & Database Management	350 Shepard Hall (3rd Fl.)
10:00 – 11:00	16:00 – 17:00	Intellectual Property (IP) Agreement & Research Facilities for Collaboration	350 Shepard Hall (3rd Fl.)
11:00 – 11:45	17:00 – 17:45	Educational Activities (Internships & Outreach)	350 Shepard Hall (3rd Fl.)
11:45 – 12:00	17:45 – 18:00	External Evaluation Review	350 Shepard Hall (3rd Fl.)
12:00 – 12:30	18:00 – 18:30	Wrap-up & Next Annual Review Meeting	350 Shepard Hall (3rd Fl.)
12:30 – 2:00	18:30 – 20:00	Lunch	Faculty Dining Room
2:00 – 3:30	20:00 – 21:30	Advanced Science Research Center (ASRC) Lab Tour	ASRC (CCNY Campus)

Appendix 2: Advisory Board meeting Agenda

1) Masahiro Kawaji: PIRE Year 1 summary (20 minutes) This will provide an overview of PIRE objectives and overall plan, as well as progress toward objectives in Year 1.

2) PIRE Thrust leaders (M. Kawaji, T. Lee, R. Messinger and J. Morris) and International Team Coordinators (L. Fournaison and H. Linga). (20 minutes) This will offer the team leadership's viewpoints and concepts of synergy.

3) Meeting with students and post-doctoral associate. (20 minutes)

4) Discussion (30 minutes)

Appendix 3:

Evaluation Report for PIRE at City College of New York: Year 1

Draft

Denis Gray, Ph.D., External Evaluator

Prepared July 15, 2018

Abstract

Consistent with its proposal, PIRE at CCNY Multi-Scale, Multi-Phase Phenomena in Complex Fluids for the Energy Industries project will participate in an evaluation by an external evaluator. The focus of this evaluation during the early stages (years 1 and 2), will be on **monitoring** and **formative evaluation** efforts. This report focuses on the implementation of the project plan and feedback from the project's first annual meeting.

In order to facilitate the ongoing evaluation of the project a logic model (Appendix 3A) was developed which graphically displays what activities will lead to various project outputs (short term), outcomes (midterm) and impacts (long term) (See Appendix A). Program documents were used to assess the extent to which various implementation activities detailed in the logic model have been planned and/or implemented to achieve project outcomes and impacts. As detailed in the report the project PIs have made tremendous progress in standing up the project in all of the project domains including: Project Management, Knowledge Advancement, Education and Training, Recruitment of Underrepresented Students, Undergraduate/High School Research Experiences. Among these areas the recruitment of the first cohort of students, beginning international collaborations, and beginning international internships appear to be outstanding examples of the implementation effort.

Another area of success was the planning and implementation of the annual PIRE meeting held in June of 2018 that was attended by 44 individuals. A feedback survey about this event was conducted and achieved an enviable 82% response rate. Feedback was provided by both U.S. and non-U.S. attendees and in-person and virtual attendees. Ratings of the usefulness of the meeting sessions were uniformly high (averaging "very useful (4/5-point scale). Most suggestions for improvement focused on the thrust sessions and indicated these sessions should be given more agenda time and become more interactive in the future. Ratings for achieving various meeting objectives (become more familiar with project scope and goals; become more familiar with research performed and planned in various thrusts; meet and network with other participants; discuss opportunities to share resources and collaborate; identify institutions for international student placements) were also rated consistently high (average rating somewhere between agreed (4) and strongly agreed (5)). Only minor suggestions for improving PIRE, its research and future meetings were provided.

While work remains in a number of areas including education and training, underrepresented recruitment and high school experiences, based on my assessment the PIRE at CCNY has had a very productive and effective first year.

Introduction

The PIRE at CCNY Multi-Scale, Multi-Phase Phenomena in Complex Fluids for the Energy Industries project (hereafter referred to as the "project) has secured my services as an external evaluator to assist in the task of documenting project activities and providing formative feedback on the success of various project processes and activities. The evaluation will focus on the achievement of the project's four objectives:

> The evaluation will focus on addressing our effectiveness in achieving four PIRE objectives:
>
> *1. Support excellence in S&E research and education through international collaboration.*
> *2. Promote opportunities where international collaboration can provide unique advantages of scope, scale, flexibility, expertise, facilities, or access to phenomena, enabling advances that could not occur otherwise.*
> *3. Engage and share resources and research infrastructure within and across institutions to build strong international partnerships.*

4. Create and promote opportunities for students and early career researchers to participate in substantive international research experiences.

The project proposal described the plans for the initial evaluation effort as follows: "The project evaluation strategy will evolve over the life cycle of the award. During the early stages (years 1 and 2), the focus will be on **monitoring** and **formative evaluation** efforts. That is, program records and direct observation will be used to assess whether key activities and interventions are implemented as intended (e.g., international collaborations; a system of joint supervision of Ph.D. students; annual international symposia; aggressive minority recruitment, etc.). Qualitative methods (e.g., interviews, focus groups) including participant observation at regular meetings, will be used to collect supplemental information from stakeholders to refine and improve collaborative research, educational and outreach activities." Later in the project, I will focus on output and outcome evaluation. Consistent with this strategy my report will focus two areas: the implementation of the project plan and feedback from the project's first annual meeting.

Implementation Assessment

The PIRE project proposal for CCNY included a detailed description of project objectives, activities, and anticipated outputs and outcomes. In order to facilitate the ongoing evaluation of the project, I prepared a detailed "logic model" as shown in Appendix 3A. The logic model attempts to graphically display what activities will lead to various project outputs (short term), outcomes (midterm) and impacts (long term) (See Appendix A). It is important to note that I anticipate the activities, goals and outcomes of this project will change over time and this document will need to be updated periodically.

My focus at this point is monitoring or project implementation activities. Based on project documents including the PIs Overview Presentation of Progress in Year 1, it is apparent the PI and his collaborators have made tremendous progress during their first year. While most of these activities are documented in the PI's annual report it is worth repeating some of these achievements here. With respect to **Project Management**: the project's steering committee, advisory board (with six members), and management team has been established; PIRE coordinator appointed; thrust leaders appointed and website created; monthly management meetings have been held; annual meeting of all stakeholders planned and held. With respect to the **Knowledge Advancement** domain: PIs and students have been assigned and begun work on the project's five thrust areas at both the molecular and macroscopic levels; collaborative activities including mini-workshop have begun; contacts and some visits have been made with international partners at all the collaborating universities (Norway, France, Germany) across all thrust areas. With respect to the **Education and Training** domain: 6 PhD and 2 MS research assistants and 1 post docs have been appointed; a small cohort of students have begun their international internships. With respect to **Recruitment of Underrepresented Students**: a partnership with LSAMP has been put in place that is coordinated with Dr. Brathwaite; some students have been recruited to work within the project with two Senior College students participating in research efforts in France during June. With respect to **Undergraduate/High School Research Experiences**: initial conversations have been held with one high school and a student recruited to begin summer research experience at CCNY this summer. As described above, for the evaluation effort: the logic model has been prepared and shared with the team, a presentation about the evaluation strategy was delivered at the annual meeting; a feedback survey was administered at the annual meeting and summarized. Importantly, project PIs have begun to present their results findings at various national and international conferences.

In short, significant progress has been made in all of the project's major activity domains.

Feedback Survey for Annual Meeting

The first annual meeting for the PIRE at CCNY Multi-Scale, Multi-Phase Phenomena in Complex Fluids for the Energy Industries project was held at CCNY on June 18-20, 2018. The meeting was attended by 44 individuals (12 attended were remote and attended the meeting virtually). The agenda is attached as Appendix B. In order to assess the extent to which the meeting achieved its various objectives I prepared a web-based survey. A link to the survey was sent to all the registered participants on the final day of the event and reminders sent on 3 subsequent occasions. The goals

of the assessment were to assess satisfaction with the meeting and solicit suggestions for improving future meetings and the project itself. The survey was completed by 36 individuals, a 82% response rate, which is incredibly high for this type of feedback survey. The survey instrument is included as Appendix C. Frequency counts and descriptive statistics of ratings were provided and open-ended comments were subjected to content analysis and organized into themes.

Respondents. With respect to respondents the results indicated that about two-thirds of the respondents (61.1%) were from U.S.-based institutions while the balance were from non-U.S. institutions. Eighty percent of the respondents participated in the meeting in-person while the balance participated virtually. About one-third of respondents were faculty researchers; another third were students or post docs; about fifteen percent were advisory board members and most of the balance held administrative and/or support roles at CCNY or the participating international universities.

Perceived Usefulness of Meeting Sessions. Respondents were asked to indicate how useful various sessions on the agenda were in "orienting and preparing you to become involved in the PIRE project". Sessions (Overview, Thrust Areas Presentations, Lab Tours, Thrust Area Meetings, Support Sessions, Advisory Board) were rated from "not useful (1)" to "extremely useful (5)". As Figure 1 reveals all of the sessions were rated positively with most ratings averaging "very useful (4). Since note everyone attended all sessions, some sessions like lab tours and support sessions, advisory board were rated by fewer respondents. The overview session received the highest rating (4.12/5.00).

Figure 1. Usefulness of Meeting Sessions

Q4: How useful were the following sessions in orienting and preparing you to become involved in the PIRE project

	1 NOT USEFUL	2 FAIRLY USEFUL	3 USEFUL	4 VERY USEFUL	5 EXTREMELY USEFUL	N/A OR UNABLE TO RATE	TOTAL	WEIGHTED AVERAGE
Overview, PIRE Status, Next Year Meeting	0.00% 0	5.88% 2	11.76% 4	44.12% 15	35.29% 12	2.94% 1	34	4.12
Thrust Area (1,2,3,4, Modeling) Sessions	0.00% 0	5.88% 2	11.76% 4	50.00% 17	23.53% 8	8.82% 3	34	4.00
Lab Tours	0.00% 0	6.25% 2	3.13% 1	37.50% 12	9.38% 3	43.75% 14	32	3.89
Trust Area Meeting (Monday 3-5 pm)	2.86% 1	5.71% 2	11.43% 4	31.43% 11	22.86% 8	25.71% 9	35	3.88
Support Sessions (Database, IP, Lab Facilities, Education)	0.00% 0	8.82% 3	5.88% 2	41.18% 14	11.76% 4	32.35% 11	34	3.83
Advisory Board	0.00% 0	0.00% 0	11.43% 4	25.71% 9	14.29% 5	48.57% 17	35	4.06

High and very consistent rating of sessions. Average rating "very useful" (4/5-point scale) - Lab tours, thrust meetings, support sessions and advisory board rated by fewer respondents

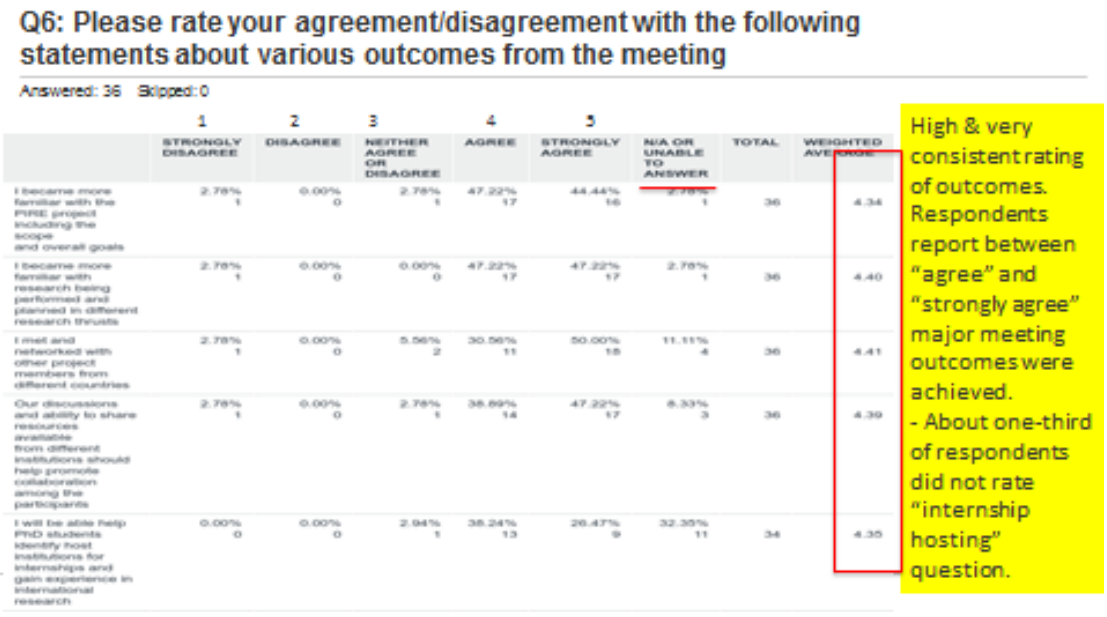
Respondents were asked to provide comments and suggestions for making the sessions more useful. As Figure 2 reveals the largest theme focused on the thrust sessions. Most of the comments suggested these sessions should be given more time and become more interactive in the future. For instance, some respondents reported, "For the thrust area meetings, time should be set aside for discussion and brainstorming"; "Presentation content from the "thrusts" could be delivered so that each topic builds off the previous one? Or the presenters could make the connection between their experiments and their colleagues' more explicit?" Some comments were also made about other sessions, ways to improve the virtual software used, and compliments for the quality of the sessions.

Figure 2. Representative Suggestions for Improving Usefulness of Sessions

Representative Comments/suggestions for how these sessions could be made more useful. (See Appendix A for all comments)
Thrust Sessions (N=8)
For the thrust area meetings, time should be set aside for discussion and brainstorming.
Stronger leadership on each thrust to avoid losing time in the definition of common work and synergies
Presentation content from the "thrusts" could be delivered so that each topic builds off the previous one? Or the presenters could make the connection between their experiments and their colleagues' more explicit?
More time is needed for each thrust meeting, and meetings shouldn't overlap each other
More discussion of the objectives and scientific questions being addressed in each thrust area
Other Sessions (N=2)
Education part is very useful because it provides students with information about how to participate in the international collaboration.
... I personally want more introduction to the computing capability of the foreign collaborators
BlueJeans (n=2)
For BlueJeans attenders, the microphone was not optimal. It seemed to react to other sounds and then stopped. Difficult to follow discussions and hear what audience said.
Compliments (N=2)
They were fine. Do not know how it should be done better. It will be even more interesting when more ongoing research will be presented in later meetings

Achievement of Meeting Objectives. The meeting was supposed to achieve five explicit objectives: become more familiar with project scope and goals; become more familiar with research performed and planned in various thrusts; meet and network with other participants; discuss opportunities to share resources and collaborate; identify institutions for international student placements. Respondents were asked to indicate whether their level of agreement/disagreement (strongly, agree, neither, disagree, strongly) with statements reflecting each of these objectives. As Figure 3 reveals respondents agreed that all of the objectives were achieved with the average rating somewhere between agreed (4) and strongly agreed (5).

Figure 3. Rating of Achievement of Meeting Objectives



Respondents were also asked to indicate how satisfied they were with the meeting planning, meals and venue arrangements. The rating for this aspect of the meeting was very high with mean rating for this question was 4.31 which was between quite satisfied (4) and extremely satisfied (5).

Suggestions for Improving PIRE and Future Meetings. Finally, respondents were asked to provide suggestions for how PIRE project, its research and future meetings could be improved. Only a few suggestions were offered. As Figure 4 reveals, with respect to future meetings some comments several minor suggestions were made about organizing a pre-meeting reception, providing more speaker and title information, and scheduling more time for technical sessions ("the level and scope of the science will increase, as well as the extent of collaborations. Thus, even more time should be blocked off for scientific discussions, including informal brainstorming sessions"). Other suggestions highlighted need to begin paying more attention to the research and training aspects of the project ("Taking into account the needs of the administration of countries hosting students, such as the need for original documents and administrative processing time").

Figure 4. Suggestions for Improving PIRE, its Research, Future Meetings

Suggestions or comments to improve the PIRE project, its research or educational activities, and/or future annual meetings.
Future Meetings (N=4)
First evening (pre-meetings) reception should be organized to enable all attendees to meet, network and get to know each other, especially students and postdocs
Schedule with pre-described presentation slots with speaker and title information
In future annual research meetings, the level and scope of the science will increase, as well as the extent of collaborations. Thus, even more time should be blocked off for scientific discussions, including informal brainstorming sessions.
Hopefully all participating institutions will be represented in future meetings
Research and Training (N=3)
It's good to send student to industrial internship as well
Taking into account the needs of the administration of countries hosting students, such as the need for original documents and administrative processing time
For research part, I hope the 6 month intern for PhD students can start soon. This will be very helpful for exchanging ideas and sharing facilities.
General (N=2)
More eagerness from everyone would be better
As of now, I do not have any comments

Appendix 3A PIRE at CCNY Logic Model

Objective	Initial monitoring and evaluation activity focus	Early outputs and outcomes	Longer-term focus
Management Structure:	• Steering Committee (SC), Advisory Board (AB) and Management Team created • Consortium Agreement established and signed • Center Coordinator appointed • Center management team created • Thrust leaders appointed • Website created	• SC, AB, MT manage the interdisciplinary research centre • Regular meetings of management teams • Annual reports submitted • Semi-annual research accomplishment reports submitted • Quarterly Newsletter prepared • Publications, budgeting and deliverables tracked • Student data base and progress records maintained	• Well managed center that initiates sustainability plan
Knowledge advancement: groundbreaking scientific discoveries in multiphase fluids research	• Implement 2 research themes (Molecular, Macroscopic), • Implement 5 research thrusts[1] • Thrust area research plans followed	• Young researchers develop interdisciplinary international skills • Networking with foreign scholars • Annual Review meetings held • Semi-annual Joint Seminars held using collaboration tools • Research disseminated in journals, conferences, and website • Researchers give guest lectures at neighboring universities	• Acquire the technical, cultural and collaborative skills to excel in an increasingly global scientific community of scholars • Breakthrough scientific discoveries • Enhancements in industrial processes and energy efficiency • Advances will be made in experimental methods and computational tools
Accelerate education and training: through	• Target undergraduates, graduates and post docs for recruitment • Implement internships	• Joint mentoring the students in research with international partners	• Students acquire the technical, cultural and collaborative skills

[1] **Research Thrusts**: Asphaltene absorption; gas hydrate slurries, Driling fluids, particle sedimentation, Phase change material energy transport and storage, modeling and simulation.

excellence and international cooperation	• Create international education experiences • Create graduate research positions • First Year PhD fellowships created • Recruiting conferences held • Additional support from CCNY • Joint supervision/mentoring program established for international internships • Undergrads provided team-based supervision & career guidance • International summer intern program established • Language preparation and cultural training courses offered • Grad and post doc offered training in advanced research tools • Short-courses/symposia offered • SINTEF in Norway, IRSTEA in France and Fraunhofer Institute in Germany will offer industrial perspective • Online learning modules developed based on project • Course on multi-scale modelling developed. • 20 high school teachers attend lab hands-on experiences	• International experiences for 10 U.S. undergraduate students • International experiences for 10 PhD students and three postdoctoral fellows trained • Students collaborate with scientists from other disciplines and backgrounds • Students participate in Annual review and semi-annual Joint Seminars • Grad and post doc develop skills in advanced research tools • Short-courses/symposia recorded and archived • Students offered summer internship???? • Online learning modules shared	to excel in an increasingly global scientific community of scholars • Students hire in industry, academe and government • Contribute to STEM workforce in US. • Students advance their research skills but also develop intercultural and team skills • Students well prepared to pursue successful careers in a global, multi-cultural environment.
Recruitment from underrepresented groups	• Partnership with LSAMP • Diversity in advisory board • Annual weekend recruiting program • LSAMP funds underrepresented students for summer research •	• Strong underrepresented participation in both undergraduate and graduate positions • Annually 2 underrepresented students funded for summer international research • Research experiences in PIRE labs	• Increased participation of underrepresented undergraduates and graduate students in STEM fields.
Provide undergraduate and high school students research experience	• Engineering Networking Reception, which will be attended by high school science teachers discuss summer research internships in CCNY labs	• Teachers attend Engineering Networking Reception • Students attend open houses	• Broadened horizons and deepening interest in pursuing

	• Open houses organized in Y1, 3, 5 • Faculty serve as judges in Science Fairs • Open houses will be held for the general public		more advanced studies in STEM disciplines
Evaluation	• Project logic model developed • Begin monitoring and formative evaluation of project implementation activities • Begin developing instruments for feedback evaluation	• Collect feedback assessments or annual review and semi-annual joint seminars • Conduct feedback assessments with students • Collect feedback from Advisory Group • International collaborative oversight" • Contribute to annual report	• Collect assessments of graduated students • Conduct bibliometric and collaboration assessments of publications • Assessment of sustainability plan • Contribute to final report