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## Preview of Award 1743794 - Annual Project Report

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### Cover

Federal Agency and Organization Element to Which Report is Submitted:	4900
Federal Grant or Other Identifying Number Assigned by Agency:	1743794
Project Title:	PIRE Investigation of Multi-Scale, Multi-Phase Phenomena in Complex Fluids for the Energy Industries
PD/PI Name:	Masahiro Kawaji, Principal Investigator Sanjoy Banerjee, Co-Principal Investigator Taehun Lee, Co-Principal Investigator Robert J Messinger, Co-Principal Investigator Jeffrey F Morris, Co-Principal Investigator
Recipient Organization:	CUNY City College
Project/Grant Period:	10/01/2017 - 09/30/2022
Reporting Period:	10/01/2019 - 09/30/2020
Submitting Official (if other than PD/PI):	N/A
Submission Date:	N/A
Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	N/A

### Accomplishments

#### \* What are the major goals of the project?

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 3, we have addressed all three major goals by setting up four Research Thrusts and a Modeling & Simulation group, all of which involve PIRE faculty and students in collaboration with 19 European researchers from eleven institutions.

**\* What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?**

Major Activities:

- Recruitment of two new PhD students (Moyosore Odunsi and Andres Velez Mendosa) replacing the PhD students who graduated with PhD degrees in 2019-2020.
- A Site Visit by NSF on September 19 and 20, 2019. In response to the review comments received from the review panel, an Interim report was submitted to NSF in February, 2020.
- Training of one postdoctoral researcher, ten PhD students, two Master's students, two undergraduate students and one high school student in PIRE research and related activities.
- Continuation of research under four Research Thrusts and Modeling & Simulation group.
- Continued research collaboration with 19 European researchers from eleven institutions in Norway, France and Germany.
- Research Thrust meetings held with collaborating researchers in Europe via a web-based meeting tool, BlueJeans, in Fall, 2019 and Spring, 2020.
- Mutual visits to discuss research, sharing of resources and enhancement of research collaboration.
- Five guest speakers invited to present expert knowledge and useful information to the PIRE researchers in PIRE seminars.
- Guest seminars recorded and video recordings made available to European collaborators through the PIRE website.
- Internship opportunity provided to one PhD student (Shaghayegh Darjani) by a Norwegian collaborator (SINTEF), however, because of COVID-19, their lab was shut down and the student had to return to the US after a short stay.

Specific Objectives:

- Continue collaborative research with European partners and promote their active involvement.
- Maintain an effective project management structure involving key personnel.
- Provide clear objectives and tasks to all the PhD students in research and related activities.
- Keep international collaborators informed of research activities underway at City College of New York and promote research collaboration through mutual visits, web-based Research Thrust meetings, Third Annual Review Meeting (postponed to a later date due to COVID-19) and hosting of PhD and undergraduate students in internships.
- Continue outreach activities by providing laboratory experiences at CCNY to one high school student.

Significant Results:

Research has continued in four Research Thrusts (Asphaltenes, Gas hydrates, Drilling fluids and Nanoemulsions) and Modeling & Simulation group with well-defined scope and research objectives.

- Twelve PhD students and one postdoctoral fellow have conducted research under different Research Thrusts. They have made progress in respective research projects and interacted with international collaborators through web-based Research Thrust meetings and mutual visits. Some of them have prepared and submitted journal papers.
- Two Master's students have been supported to work on Database development and PIRE website.
- Two undergraduate have gained laboratory experience.
- The Third Annual Review Meeting was to be hosted by French collaborators at ENSTA Paris and INRAE (formerly IRSTEA) in Paris on June 24-26, 2020, to promote international collaboration in PIRE research and sharing of scientific knowledge and resources. However, due to a COVID-19 pandemic, this meeting could not be held as planned and has been postponed until late January, 2021.
- In addition to the PIRE faculty and PhD students from CCONY, all French collaborators from Toulouse and Paris, and many collaborators from Norway and Germany were planning to attend this Annual Review Meeting.

Key outcomes or Other achievements:

PIRE researchers have made substantial progress in their research projects as summarized below.

**Dinesh K. Kalaga** is a postdoctoral researcher who has been working on drilling fluids. He has developed a Taylor-Couette cell and measured the sedimentation of Barite particles under rotational shear using Gamma densitometry, X-ray attenuation, hydrostatic pressure difference and optical probe methods. He has also performed PIV measurements to determine the liquid flow patterns and particle settling velocity under different rotational shear rates. He has continued to perform rheological measurements of actual drilling fluid samples and his journal paper co-authored with Norwegian collaborators from NTNU and SINTEF has been accepted.

**Manizheh Ansari** completed her Ph.D. study in August, 2019, and continued to investigate the microstructure and rheology of drilling fluids until February, 2020. She used Cryo-SEM and Cryo-EDS methods to image the spatial structure of the drilling fluid at nanometer to micrometer scales. She also performed rheological measurements over different shear rates. She has submitted a journal paper on her work.

**Geng Liu** is a Ph.D. student studying the simulation of multiphase flows using a lattice Boltzmann method, and the diffuse bounce back lattice Boltzmann approach for recovering the classic no slip boundary condition in diffuse geometry. He did his internship in Prof. Mathias Krause's laboratory at KIT in Germany and continued his work using OpenLB as both a user and developer. He has applied his new fluid-solid interaction model to particle flows to study the behavior of a particle in Couette flow and Taylor Couette flows.

**Shaghayegh Darjani** is a Ph.D. student studying the equation of state of a 2D hard-core lattice gas with a new numerical method based on random sequential adsorption incorporating surface diffusion (RSAD) to obtain both phase transition and adsorption kinetics. She has worked closely with Dr. Aude Simon at LCPQ in France and analyzed the interfacial behavior of asphaltenes at the water/oil interface. She has also performed Molecular Dynamics simulations to gain an insight into the adsorption of asphaltene molecules at oil/water interfaces and some experimental observations. She has published her work in the Journal of Chemical Physics and also submitted two more papers to the same Journal.

**Fang Liu** completed her PhD study in Fall, 2019. She developed a methodology to predict asphaltenes adsorption behavior, which is of great theoretical interest in upstream engineering for the oil industry. She has worked closely with our collaborators at SINTEF in Norway, studying the mixture dynamics and isotherms of asphaltenes by developing a physical model based on mixture effects. She was able to extract the properties of each pseudo-subtraction from dynamic interfacial tension measurements.

Following her industrial internship at ExxonMobil, she worked on identifying the deposition conditions for asphaltenes during crude oil recovery, by using a quartz crystal microbalance. She has published one journal paper and submitted two journal papers.

**Artur Zych** and **Jungeun Park** are Ph.D. students studying PCM Nanoemulsions: how to synthesize stable nanoemulsions to be used for effective heat storage and transport. They synthesized stable nanoemulsions of octadecane using different varieties and concentrations of surfactants and also determined the size distributions of PCM particles which can have large influences on the flow and heat transfer characteristics. Artur has constructed a heat transfer loop to test the flow and convection heat transfer characteristics of PCM Nanoemulsions. Jungeun has focused her research on NMR spectroscopy to obtain molecular-level information on the local environments, compositions, and dynamics of the oil and surfactant species from solution-state  $^1\text{H}$  and  $^{13}\text{C}$  NMR measurements.

**Fanny Thomas** is a Ph.D. student who has studied the wetting phenomena which are believed to play a crucial role in the formation and control of gas hydrates slurries. She studied the dynamics of capillary bridges and the motion of the three-phase contact line within the framework of the diffuse interface theory. Fanny successfully completed her PhD thesis and graduated in April, 2020. In December, 2019, she submitted a journal paper written jointly with Prof. D. Dalmazzone of ENSTA Paris.

**Yu Han** is a Ph.D. student working 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. His initial work has developed a boundary-integral method for axisymmetric drops, which has been applied to examine the effects of interfacial elasticity and viscosity on the deformation of asphaltene-laden interfaces.

**Dennis Burgner** is a Ph.D. student working on the properties of hydrate-forming emulsions. His work is initially focused on an experimental study coupled with a modeling project exploring a fractal aggregation model for the structure and rheology of the hydrate slurry. A feature that links his work with other PIRE projects is the role of residual water and wetting properties of the hydrate on the forces between hydrate particles.

**Chunheng Zhao** is a Ph.D. student working on the development of ternary lattice Boltzmann method with the applications to PCM nanoemulsions and/or drilling fluids. The new conservative phase field model for Lattice Boltzmann method is proposed and applied to several benchmark, like wetting problem and rising bubble problems. The new model also performs great on simulation of double emulsion problems which give rise to oil drilling modeling. The ternary fluids including oil/water/clay or weighting agent and oil/water/surfactants are also investigated, which require different modeling approaches.

**Andres Velez Mendoza** is a new PhD student in Mechanical Engineering who has been recruited to the PIRE project in Spring, 2020. He has replaced Itung Chen who withdrew from the PhD program at the end of Fall, 2019. Andres has been advised by M. Kawaji and started reviewing the drilling fluids literature. He has also been learning the operation of a Taylor-Couette cell and various measurement methods from D. Kalaga after our laboratories have been re-opened in July, 2020.

**Moyosore Odunsi** is a Physics PhD student who is studying wetting dynamics experimentally, using a combination of force measurement and visualization to explore the hysteresis in cyclic wetting of liquid contained between two surfaces. This work will be continued and coupled with numerical analysis of the problem over the next year with a goal to develop a model of the wetting of surfaces relevant to particles joined by liquid bridges, as found in capillary suspensions [E. Koos, 2014, Current Opinion in Colloid and Interface Science, 19(6):575–584] and postulated as basic to the rheology

of hydrate slurries [G. Zyliftari, J. W. Lee & J. F. Morris 2013 Chem. Eng. Sci. 95, 148-160].

**Master's Students:** We have provided two Master's students opportunities to gain experiences in the development of a PIRE Project database and website. Yamile Patino Vargas from Computer Science and Carlos Tavarez from Data Science & Engineering were supported. Yamile and Carlos completed their studies and graduated in Fall, 2019 and Spring, 2020, respectively.

**Undergraduate Internship Students:** Alejandro Varela returned from a summer internship at IRSTEA in France in August, 2019, and worked on a heat transport flow loop for PC Nanoemulsions. Itung Chen completed a summer internship at NTNU/SINTEF in Norway in the summer of 2019 working on a drilling fluids project.

**High School Student:** Christopher Silva from Ossining High School in New York conducted research in the summer of 2019. He was able to present his work on drilling fluids at the Westchester/Rochester Junior Science and Humanities symposium and earned a 2nd place in the category of engineering.

### \* What opportunities for training and professional development has the project provided?

#### International Collaboration

Many opportunities have been created to enable PIRE Project faculty and students to interact and collaborate with international researchers through web-based Research Thrust meetings, Second Annual Review Meeting, and mutual visits as summarized below.

Research Thrust meetings were held with international collaborators in all four Thrusts and Modeling & Simulation Group in November-December, 2018 and April-June, 2019. Each meeting was about two hours in duration and presentations were made by both CCNY researchers and European collaborators as shown below.

Thrust 1 -Asphaltenes: January 27th, 2020

- Fang Liu, CCNY - "Mixture Effects in Asphaltene Absorption at Liquid-Liquid Interfaces", and "Study of Asphaltene Deposition on Solid Surfaces"
- Shaghayegh Darjani, CCNY "Molecular dynamics study of adsorption of asphaltenes at Oil/water interface"
- Martin Fossen, SINTEF, "Plans for Shaghayegh Darjani's Asphaltene Research in Norway – Direct Fractionation of Asphaltenes and Subsequent Characterization"

Thrust 2 - Gas Hydrates: January 24, 2020

- Jeff Morris, CCNY: 2020 planning - Initiation of a Thrust objective: Process/Flow Assurance Synergy
- Didier Dalmazzone, ENSTA Paris: "MUSCOFI update and an introduction"
- Martin Fossen, SINTEF: "Update and some recent results"
- Sebastien Teychéne / Raj Ramamoorthy, LGC: 2020 Plans -- "crystallization experiments"
- General discussion -- Aude Simon provided issues on which she hopes for some guidance, regarding the type of hydrates best for study by the DFTB method, as well as the type of data that would be the goal.

Thrust 3 - Drilling Fluids: Nov. 25, 2019

- Masahiro Kawaji, CCNY: "Summary of NSF Site Visit"
- Bjornar Lund, SINTEF: "Research and publication plans"
- Titus Ofei, NTNU: "Influence of static and dynamic conditions on Barite sag and stability in OBM: experimental results"
- Blandine Feneuil, Univeristy of Oslo: "Study of sedimentation of particles in emulsions"
- Dinesh Kalaga, CCNY: "Sedimentation of weighting material and drilling fluid's rheology"

Thrust 4 - PCM Nanoemulsions: originally planned in early December, but then postponed to the Spring semester, 2020.

Modeling & Simulation Group: originally planned in early December, but then postponed to the Spring semester, 2020.

**PIRE Project Integration Meeting, January 28, 2020**

The purpose of this meeting was to identify and discuss common issues of interest to all the Research Thrusts in PIRE, such as wetting and interfacial properties. All the PIRE faculty and most of PhD students attended this meeting to observe actual fluid samples investigated in various Thrusts. The first meeting was focused on the wetting phenomena which play a significant role in the formation and behavior of gas hydrates and other complex fluids.

### **Group meetings**

In each Thrust, group meetings have been held by the PIRE faculty and PhD students. For example, in the PCM Nanoemulsions Thrust, two faculty (M. Kawaji and R. Messinger) and two PhD students (A. Zych and J. Park) met on November 1 and December 18, 2019, to discuss research progress and future plans.

### **Interactions with Collaborators in France, Norway and Germany.**

Two undergraduate students gained summer internship experiences in Norwegian and French collaborators' laboratories. Itung Chen spent two months at NTNU/SINTEF in Trondheim, Norway, studying the techniques used to synthesize and characterize the oil-based drilling fluids. Alejandro Valera spent two months at IRSTEA in Paris to perform experiments on gas hydrates using a gas hydrate flow loop. He learned the operation of the flow loop and measurement techniques.

In addition, the following interaction was made by PIRE faculty, students, and collaborating researchers.

Co-PI Messinger and Ph.D. student Jay Park met Dr. Ulrich Scheler at the ENC conference in Baltimore, MD, in March 2020, to discuss research related to the Phase Change Material Nanoemulsion thrust, as well as Park's upcoming internship in Germany, which will occur in 2021. Dr. Scheler also agreed to serve as a member of Park's Ph.D. committee.

### **Guest Seminars**

Three guest seminars were organized to share expert knowledge and useful information with PIRE researchers before the campus was shut down in March, 2020.

- October 15, 2019, Prof. Chris Boyce of Columbia University gave a seminar entitled "MRI and Computational Modeling of Multiphase Flow Systems".
- November 21, 2019: Prof. Rigoberto Morales from the University of Parana in Brazil gave a talk on modelling and experimental research on multiphase flows in pipes with hydrate formation.
- February 10th, 2020, Prof. Siyoung Choi, from KAIST, gave a seminar entitled "Fluid/fluid interface engineering and its energy applications.

### **Independent Evaluation**

Prof. Denis Gay of North Carolina State University has evaluated the progress made by CCNY's PIRE Team in the third year of this PIRE project. His evaluation report is attached as Appendix 3 and includes an evaluation of program implementation, student experiences in research, interactions with international collaborators, and scholarly publications.

### **\* How have the results been disseminated to communities of interest?**

In Year 3, some results from our PIRE research have been submitted, accepted or published in journals and presented in conference papers in collaboration with researchers in France and Norway as summarized below.

### **Journal papers published or accepted:**

Darjani, S., Koplik, J., Banerjee, S., Pauchard, V., 2019. Liquid-Hexatic-Solid Phase Transition of a Hard-Core Lattice Gas with Third Neighbor Exclusion", J. Chem. Phys. 151, 104702 (2019) <https://doi.org/10.1063/1.5123231>

Liu, F., Hickman S., Maqbool T., Pauchard, V. & Banerjee, S., 2020. Study of asphaltene depositions onto stainless steel surfaces using quartz crystal microbalances with dissipation. Published in Energy & Fuels. <https://pubs.acs.org/action/showCitFormats?doi=10.1021/acs.energyfuels.0c00663&ref=pdf>

Schuler, B., Zhang, Y., Liu, F., Pomerantz, A.E., Andrews, A.B., Gross, L., Pauchard, V., Banerjee, S., and Mullins, O.C., 2020. Overview of Asphaltene Nanostructures and Thermodynamic Applications, Energy & Fuels, American Chemical Society. <https://doi.org/10.1021/acs.energyfuels.0c00874>

Baroudi L., Lee, T., 2020. Effect of Interfacial Mass Transport on Inertial Spreading of Liquid Droplets, Physics of Fluids 32, 032101. <https://doi.org/10.1063/1.5135728>

Ofei, T. N., Kalaga, D., Lund, B., Saasen, A., Linga, H., Sangesland, S., Gyland, R. K. and Kawaji, M., 2020. Laboratory Evaluation of Static and Dynamic Sag in Oil-Based Drilling Fluids, Paper SPE-199567-PA accepted for publication in SPE Journal.

### **Journal papers submitted and under review.**

Darjani, S., Koplik, J., Pauchard, V., Banerjee, S., Role of Surface Diffusion and Desorption on Surface Crowding of the Honeycomb Lattice, submitted to J. Chem. Phys., July 2020.

Chan, T. S., Pedersen, C., Koplik J., Carlson, A., Film deposition and dynamics of a self-propelled wetting droplet on a cone with slip, under review for publication in J. Fluid Mech. (2020).

Thomas, L.F., Morris, J.F., and Dalmazzone, D. Contact angle measurements on cyclopentane hydrates, submitted to Chemical Engineering Science (a revised paper under review).

Ansari, M., Turney, D., Morris, J., Banerjee, S., Investigations of rheology and a link to microstructure of oil-based drilling fluids, submitted to Journal of Petroleum Science and Engineering (a revised paper under review).

Liu G., Lee, T. Diffuse Bounce-back Condition for Lattice Boltzmann Method, submitted to Computers & Fluids.

Baroudi L., Lee, T. Simulation of a Bubble Rising at High Reynolds Number with Mass-conserving Finite Element Lattice Boltzmann Method, submitted to Computers & Fluids.

Liu, F., Banerjee, S., & Pauchard, V. Modelling the multicomponent compositional effects of asphaltenes on interfacial phenomena, submitted to Energy & Fuels in July, 2020.

### **Journal papers under preparation for submission by September, 2020.**

Darjani, S., Koplik, J., Pauchard, V. and Banerjee, S. "Adsorption kinetics and Equation of State of Binary Mixture of Hard Core Particles on a Square Lattice" to be submitted to J. Chem. Phys. in August, 2020.

Thomas, L.F., Lee, T., Morris, J.F., "Capillary stress tensor method for contact line dynamics in the diffuse interface method", to be submitted to Physical Review Fluids in September, 2020.

### **Conference Papers and Presentations:**

Ansari M., Kalaga D.V., Turney D.E., Morris, J., Banerjee S., Kawaji M., Microstructure and rheological properties of oil-based drilling fluids, AIChE Annual Meeting, Orlando, Florida, USA, November 10 -15, 2019.

Kalaga D.V., Ansari M., Banerjee S., Kawaji M., Gyland K.R., Lund B., Settling characteristics of weighting material in the oil-based drilling fluids, AIChE Annual Meeting, Orlando, Florida, USA, November 10 -15, 2019.

Darjani, S., Pauchard, V., Banerjee, S., Koplik, J., Steric hindrance effect on adsorption kinetics of asphaltenes on oil/water interfaces, AIChE Annual Meeting, Orlando, Florida, November 10 -15, 2019.

T. Lee, "Fully Implicit Force Splitting Scheme to Two-phase Lattice Boltzmann Equation in Pressure-velocity Formulation," The 72nd Annual Meeting of the American Physical Society / Division of Fluid Dynamics, Seattle, WA, USA, Nov. 23–26 (2019)

Messinger, R., "Molecular-level insights into the charge storage mechanism of rechargeable aluminum batteries reveals by solid-state NMR spectroscopy," Experimental Nuclear Magnetic Resonance Conference (ENC), 09-13 March 2020, Baltimore, MD.

Park, J., "Molecular-Level Understanding of Phase Stability in Octadecane-Water-Stearic Acid Phase-Change Nano-emulsions for Thermal Energy Storage," Experimental Nuclear Magnetic Resonance Conference (ENC), 09-13 March 2020, Baltimore, MD.

### **Thesis/Dissertations**

Manizheh Ansari, 2019. "Intensification of Gas Absorption in a Downward Flow Microbubble Bioreactor", PhD Thesis, Chemical Engineering Department, City College of New York.

Fang Liu, 2019. "Understanding Asphaltenes Adsorption at Liquid-Liquid Liquid-Solid Interfaces", PhD Thesis, Chemical Engineering Department, City College of New York.

Fanny Thomas, 2020. "Capillary forces and wetting dynamics by diffuse-interface modeling", PhD Thesis, Chemical Engineering Department, City College of New York.

### PIRE Website

To help disseminate information on the CCNY-PIRE Project to the research community and general public, the PIRE projects website was developed by Yamile Vargas, a Computer Science Master's student.

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

This website was opened to the public in May 2018, and has links to the researchers' home pages 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.

### \* What do you plan to do during the next reporting period to accomplish the goals?

- At least four out of six PhD students who started in Fall, 2017, would graduate by the end of Year 3. Four new PhD students recruited in Year 2 will continue the research work under the four Research Thrusts and Modeling & Simulation Group.
- in the summer of 2021, two PhD students and two undergraduate students will be sent to Europe to experience research internships in collaborators' laboratories. Two high school students will be recruited to experience summer internships in PIRE Project laboratories at CCNY.
- Ph.D. students will continue to submit and publish their work in Journals and make presentations in conferences and technical meetings. Many of these papers will be prepared jointly with European collaborators.
- Our research activities in Year 3 were somewhat affected by a recent COVID-19 pandemic as described in Appendix 1, but the future plans have not changed. Our collaborators' laboratories were also closed in March-May, 2020, due to the COVID-19 pandemic, but they have resumed their research activities and their research plans are briefly described in Appendix 2.

### Supporting Files

Filename	Description	Uploaded By	Uploaded On
Appendix 1 CCNY's Response to the NSF Questions on PIRE - COVID 19 Fall Out.pdf	CCNY's Response to NSF's Questionnaire on COVID-19 Fall Out	Masahiro Kawaji	07/28/2020
Appendix 2 Activities and Future Plans of PIRE Collaborators in Norway and France.pdf	Activities and Future Plans of PIRE Collaborators in Norway and France	Masahiro Kawaji	07/28/2020
Appendix 3 Report by an Independent Evaluator.pdf	PIRE Evaluation Report by an Independent Evaluator	Masahiro Kawaji	07/29/2020

## Products

### Books

### Book Chapters

### Inventions

### Journals or Juried Conference Papers

View all journal publications currently available in the [NSF Public Access Repository](#) for this award.



The results in the NSF Public Access Repository will include a comprehensive listing of all journal publications recorded to date that are associated with this award.

Darjani, Shaghayegh and Koplik, Joel and Banerjee, Sanjoy and Pauchard, Vincent. (2019). Liquid-hexatic-solid phase transition of a hard-core lattice gas with third neighbor exclusion. *The Journal of Chemical Physics*. 151 (10) 104702. Status = Deposited in NSF-PAR [doi:10.1063/1.5123231](https://doi.org/10.1063/1.5123231) ; Federal Government's License = Acknowledged. (Completed by Kawaji, Masahiro on 07/28/2020 ) [Full text](#) [Citation details](#)

Baroudi, Lina and Lee, Taehun. (2020). Effect of interfacial mass transport on inertial spreading of liquid droplets. *Physics of Fluids*. 32 (3) 032101. Status = Deposited in NSF-PAR [doi:10.1063/1.5135728](https://doi.org/10.1063/1.5135728) ; Federal Government's License = Acknowledged. (Completed by Kawaji, Masahiro on 07/28/2020 ) [Full text](#) [Citation details](#)

Kalaga, D. V.. (2019). Settling of barite particles in oil-based drilling fluids. *10th International Conference on Multiphase Flow, ICMF 2019*. . Status = Deposited in NSF-PAR Federal Government's License = Acknowledged. (Completed by Kawaji, Masahiro on 08/02/2019 ) [Full text](#) [Citation details](#)

Darjani, Shaghayegh and Koplik, Joel and Pauchard, Vincent. (2017). Extracting the equation of state of lattice gases from random sequential adsorption simulations by means of the Gibbs adsorption isotherm. *Physical Review E*. 96 (5) . Status = Deposited in NSF-PAR [doi:10.1103/PhysRevE.96.052803](https://doi.org/10.1103/PhysRevE.96.052803) ; Federal Government's License = Acknowledged. (Completed by Kawaji, null on 07/31/2018 ) [Full text](#) [Citation details](#)

Liu, F., Hickman S., Maqbool T., Pauchard, V. & Banerjee, S., 2020. Study of asphaltene depositions onto stainless steel surfaces using quartz crystal microbalances with dissipation. Published in *Energy & Fuels*.  
<https://pubs.acs.org/action/showCitFormats?doi=10.1021/acs.energyfuels.0c00663&ref=pdf>. Status = ACCEPTED.

Darjani, S., Koplik, J., Pauchard, V., Banerjee, S., Role of Surface Diffusion and Desorption on Surface Crowding of the Honeycomb Lattice, submitted to *J. Chem. Phys.*, July 2020.. Status = SUBMITTED.

Chan, T. S., Pedersen, C., Koplik J., Carlson, A., Film deposition and dynamics of a self-propelled wetting droplet on a cone with slip, under review at *J. Fluid Mech.* (2020).. Status = SUBMITTED.

Thomas, LF., Morris, J.F., and Dalmazzone, D. Contact angle measurements on cyclopentane hydrates, submitted to *Chemical Engineering Science* (a revised paper under review).. Status = UNDER\_REVIEW.

Ofei, T. N., Kalaga, D., Lund, B., Saasen, A., Linga, H., Sangesland, S., Gyland, R. K. and Kawaji, M., 2020. Laboratory Evaluation of Static and Dynamic Sag in Oil-Based Drilling Fluids, submitted to *SPE Journal* (a revised paper under review).. Status = ACCEPTED.

Ansari, M., Turney, D., Morris, J., Banerjee, S., Investigations of rheology and a link to microstructure of oil-based drilling fluids, submitted to *Journal of Petroleum Science and Engineering* (a revised paper under review).. Status = UNDER\_REVIEW.

Liu G., Lee, T. Diffuse Bounce-back Condition for Lattice Boltzmann Method, submitted to *Computers & Fluids*.. Status = SUBMITTED.

Baroudi L., Lee, T. Simulation of a Bubble Rising at High Reynolds Number with Mass-conserving Finite Element Lattice Boltzmann Method, submitted to *Computers & Fluids*.. Status = SUBMITTED.

Liu, F., Banerjee, S., & Pauchard, V. Modelling the multicomponent compositional effects of asphaltene on interfacial phenomena, submitted to *Energy & Fuels* in July, 2020.. Status = SUBMITTED.

Schuler, B., Zhang, Y., Liu, F., Pomerantz, A.E., Andrews, A.B., Gross, L., Pauchard, V., Banerjee, S., and Mullins, O.C., 2020. Overview of Asphaltene Nanostructures and Thermodynamic Applications, *Energy & Fuels*, American Chemical Society. <https://doi.org/10.1021/acs.energyfuels.0c00874>. Status = ACCEPTED.

## Licenses

### Other Conference Presentations / Papers

Lee, T. (2019). *Fully Implicit Force Splitting Scheme to Two-phase Lattice Boltzmann Equation in Pressure-velocity Formulation*. The 72nd Annual Meeting of the American Physical Society / Division of Fluid Dynamics. Seattle, WA, USA.

Status = PUBLISHED; Acknowledgement of Federal Support = No

Ansari M., Kalaga D.V., Turney D.E., Morris. J., Banerjee S., Kawaji M. (2019). *Microstructure and rheological properties of oil-based drilling fluids*. AIChE Annual Meeting. Orlando, Florida, USA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Park, J. (2020). *Molecular-Level Understanding of Phase Stability in Octadecane-Water-Stearic Acid Phase-Change Nano-emulsions for Thermal Energy Storage*. Experimental Nuclear Magnetic Resonance Conference (ENC). Baltimore, MD. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Messinger, R. (2020). *Molecular-level insights into the charge storage mechanism of rechargeable aluminum batteries reveals by solid-state NMR spectroscopy*. Experimental Nuclear Magnetic Resonance Conference (ENC). Baltimore, MD. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Kalaga D.V., Ansari M., Banerjee S., Kawaji M., Gyland K.R., Lund B. (2019). *Settling characteristics of weighting material in the oil-based drilling fluids*. AIChE Annual Meeting. Orlando, Florida, USA. Status = PUBLISHED; Acknowledgement of Federal Support = No

Darjani, S., Pauchard, V., Banerjee, S., Koplik, J. (2019). *Steric hindrance effect on adsorption kinetics of asphaltenes on oil/water interfaces*. AIChE Annual Meeting. Orlando, Florida. Status = PUBLISHED; Acknowledgement of Federal Support = No

## Other Products

## Other Publications

## Patents

## Technologies or Techniques

## Thesis/Dissertations

Fanny Thomas. *Capillary forces and wetting dynamics by diffuse-interface modeling*. (2020). City College of New York. Acknowledgement of Federal Support = Yes

Manizheh Ansari. *Intensification of Gas Absorption in a Downward Flow Microbubble Bioreactor*. (2019). City College of New York. Acknowledgement of Federal Support = Yes

Fang Liu. *Understanding Asphaltenes Adsorption at Liquid-Liquid Liquid-Solid Interfaces*. (2019). City College of New York. Acknowledgement of Federal Support = Yes

## Websites

### Supporting Files

Filename	Description	Uploaded By	Uploaded On
Fang Liu et al. Energy & Fuels proof read only.pdf	Liu, F., Hickman S., Maqbool T., Pauchard, V. & Banerjee, S., 2020. Study of asphaltenes depositions onto stainless steel surfaces using quartz crystal microbalances with dissipation. Published in Energy & Fuels. <a href="https://pubs.acs.org/action/showCitFormats?doi=10.1021/acs.energyfuels.0c00663&amp;ref=pdf">https://pubs.acs.org/action/showCitFormats?doi=10.1021/acs.energyfuels.0c00663&amp;ref=pdf</a>	Masahiro Kawaji	07/27/2020
SPE Journal_Final.pdf	Ofei T. et al. 2020. Laboratory Evaluation of Static and Dynamic Sag in Oil-Based Drilling Fluids, accepted for publication in SPE Journal.	Masahiro Kawaji	07/28/2020
Baroudi and Lee Physics of Fluids 2020.pdf	Baroudi L., Lee, T., 2020. Effect of Interfacial Mass Transport on Inertial Spreading of Liquid Droplets, Physics of Fluids 32, 032101. <a href="https://doi.org/10.1063/1.5135728">https://doi.org/10.1063/1.5135728</a>	Masahiro Kawaji	07/28/2020

Filename	Description	Uploaded By	Uploaded On
Darjani et al Journal of Chemical Physics 2020.pdf	Darjani, S., Koplik, J., Banerjee, S., Pauchard, V., 2019. Liquid-Hexatic-Solid Phase Transition of a Hard-Core Lattice Gas with Third Neighbor Exclusion", J. Chem. Phys. 151, 104702 (2019) <a href="https://doi.org/10.1063/1.5123231">https://doi.org/10.1063/1.5123231</a>	Masahiro Kawaji	07/28/2020

## Participants/Organizations

### What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Kawaji, Masahiro	PD/PI	3
Banerjee, Sanjoy	Co PD/PI	1
Lee, Taehun	Co PD/PI	1
Messinger, Robert	Co PD/PI	1
Morris, Jeffrey	Co PD/PI	1
Koplik, Joel	Co-Investigator	1

### Full details of individuals who have worked on the project:

#### Masahiro Kawaji

**Email:** [kawaji@me.ccny.cuny.edu](mailto:kawaji@me.ccny.cuny.edu)

**Most Senior Project Role:** PD/PI

**Nearest Person Month Worked:** 3

**Contribution to the Project:** Directed the CCNY-PIRE Project as a PI. Leader of the PCM Nanoemulsions Research Thrust. Supervised a postdoctoral fellow and two PhD students. Organized Research Thrust meetings, Second Annual Review Meeting, Guest seminars, PhD student internships, undergraduate and high school summer student internships. Prepared the Year 3 Annual Report.

**Funding Support:** None.

**International Collaboration:** Yes, Norway

**International Travel:** No

#### Sanjoy Banerjee

**Email:** [banerjee@ccny.cuny.edu](mailto:banerjee@ccny.cuny.edu)

**Most Senior Project Role:** Co PD/PI

**Nearest Person Month Worked:** 1

**Contribution to the Project:** Leader of the Drilling Fluids Research Thrust and supervised three PhD students under Asphaltenes and Drilling Fluids Thrusts and Modeling & Simulation Group.

**Funding Support:** None.

**International Collaboration:** Yes, Norway

**International Travel:** No

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**Taehun Lee****Email:** thlee@ccny.cuny.edu**Most Senior Project Role:** Co PD/PI**Nearest Person Month Worked:** 1**Contribution to the Project:** Leader of Modeling & Simulation Group, supervised two PhD students, participated in Research Thrust meetings and Second Annual Review Meeting.**Funding Support:** None.**International Collaboration:** Yes, Germany**International Travel:** No

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**Robert J Messinger****Email:** rmessinger@ccny.cuny.edu**Most Senior Project Role:** Co PD/PI**Nearest Person Month Worked:** 1**Contribution to the Project:** Leader of the Asphaltenes Research Thrust. Supervised two PhD students under collaboration with a German researcher.**Funding Support:** None.**International Collaboration:** Yes, Germany**International Travel:** No

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**Jeffrey F Morris****Email:** morris@ccny.cuny.edu**Most Senior Project Role:** Co PD/PI**Nearest Person Month Worked:** 1**Contribution to the Project:** Co-PI and a Leader of Gas Hydrates Research Thrust. Supervised two PhD students under Gas Hydrates Thrust, participated in Thrust meetings and Second Annual Meeting, and organized a Project Integration meeting.**Funding Support:** None.**International Collaboration:** Yes, France**International Travel:** No

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**Joel Koplik****Email:** jkoplik@ccny.cuny.edu**Most Senior Project Role:** Co-Investigator**Nearest Person Month Worked:** 1**Contribution to the Project:** Supervised two PhD students at City College of New York, attended Research Thrust meetings and Second Annual Review Meeting.**Funding Support:** None**International Collaboration:** Yes, Norway**International Travel:** No

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**What other organizations have been involved as partners?**

<b>Name</b>	<b>Type of Partner Organization</b>	<b>Location</b>
Fraunhofer Institute ISE	Other Organizations (foreign or domestic)	Freiburg, Germany
Karlsruhe Institute of Technology (KIT)	Academic Institution	Karlsruhe, Germany
University of Oslo (UIO)	Academic Institution	Oslo, Norway
École Nationale Supérieure de Techniques Avancées	Academic Institution	Paris, France
Laboratoire de Chimie et Physique Quantiques (LCPQ)	Academic Institution	Toulouse, France
Leibniz Institut für Polymerforschung Dresden e.V. (IPF)	Other Organizations (foreign or domestic)	Dresden, Germany
National Polytechnic Institute of Toulouse (INP-ENSIACET)	Academic Institution	Toulouse, France
National Research Inst. of Science & Technology (INRAE)	Other Organizations (foreign or domestic)	Paris, France
Norwegian Foundation for Scientific & Industrial Research	Other Organizations (foreign or domestic)	Trondheim, Norway
Norwegian University of Science and Technology (NTNU)	Academic Institution	Trondheim, Norway
Ruhr-Universität Bochum (RUB)	Academic Institution	Oberhausen, Germany
University of Hamburg (UH)	Academic Institution	Hamburg, Germany

#### **Full details of organizations that have been involved as partners:**

##### **Fraunhofer Institute ISE**

**Organization Type:** Other Organizations (foreign or domestic)

**Organization Location:** Freiburg, Germany

**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in PCM Nanoemulsions

##### **Karlsruhe Institute of Technology (KIT)**

**Organization Type:** Academic Institution

**Organization Location:** Karlsruhe, Germany

**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in Modeling and Simulation

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#### **Laboratoire de Chimie et Physique Quantiques (LCPQ)**

**Organization Type:** Academic Institution

**Organization Location:** Toulouse, France

**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in Modeling and Simulation

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#### **Leibniz Institut für Polymerforschung Dresden e.V. (IPF)**

**Organization Type:** Other Organizations (foreign or domestic)

**Organization Location:** Dresden, Germany

**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in PCM Nanoemulsions

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#### **National Polytechnic Institute of Toulouse (INP-ENSIACET)**

**Organization Type:** Academic Institution

**Organization Location:** Toulouse, France

**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in two Research Thrusts 2 and 4 – Asphaltenes and Gas hydrates

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#### **National Research Inst. of Science & Technology (INRAE)**

**Organization Type:** Other Organizations (foreign or domestic)

**Organization Location:** Paris, France

**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in two Research Thrusts 2 and 4 – Gas hydrates and PCM Nanoemulsions

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#### **Norwegian Foundation for Scientific & Industrial Research**

**Organization Type:** Other Organizations (foreign or domestic)

**Organization Location:** Trondheim, Norway

**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in two Research Thrusts 1 and 3 - Asphaltenes and Drilling fluids

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**Norwegian University of Science and Technology (NTNU)****Organization Type:** Academic Institution**Organization Location:** Trondheim, Norway**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in two Research Thrusts 1 and 3 - Asphaltenes and Drilling fluids

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**Ruhr-Universität Bochum (RUB)****Organization Type:** Academic Institution**Organization Location:** Oberhausen, Germany**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in Gas hydrates

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**University of Hamburg (UH)****Organization Type:** Academic Institution**Organization Location:** Hamburg, Germany**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in Modeling and Simulation

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**University of Oslo (UIO)****Organization Type:** Academic Institution**Organization Location:** Oslo, Norway**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in two Research Thrusts 1 and 3 - Asphaltenes and Drilling fluids

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**École Nationale Supérieure de Techniques Avancées****Organization Type:** Academic Institution**Organization Location:** Paris, France**Partner's Contribution to the Project:**

Collaborative Research

**More Detail on Partner and Contribution:** Research collaboration in two Research Thrusts 2 and 4 – Gas hydrates and PCM Nanoemulsions

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**What other collaborators or contacts have been involved?**

**Postdoctoral fellow** at CCNY: Dinesh Kalaga

**PhD students** at CCNY: Manizheh Ansari, Dennis Burgner, Shaghayegh Darjani, Yu Han, Fang Liu, Geng Liu, Jungeun Park, Fanny Thomas, Chunheng Zhao, Artur Zych, Andres Velez Mendosa, and Moyosore Odunsi

**Master's students** at CCNY: Carlos Tavarez and Yamile Patino Vargas

**Project Coordinator** at CCNY: Sumer Mishue

**Project Assistant** at CCNY: Alice Chung

**Internal Advisor:** John Tsapogas, Director of the RF Office of Award Pre-Proposal Support

**Undergraduate student interns** at CCNY: Alejandro Varela and Itung Chen

**High School student intern:** Christopher Silva from Ossining High School

**External Evaluator:** Denis Gray, Professor at North Carolina State University

**Advisory Board members:** Morton Denn (Emeritus Professor of City College of New York), Lamia Goual (Associate Professor of University of Wyoming), Oliver Mullins (Schlumberger Fellow), George Hirasaki (Rice University) and Harald Kallevic (Equinor researcher in Norway).

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## Impacts

### What is the impact on the development of the principal discipline(s) of the project?

The principal discipline that would be impacted by this PIRE project is Complex Fluids which is a sub-discipline of Fluid Mechanics. We have been conducting international research to advance the knowledge of multi-scale phenomena in complex (Non-Newtonian), multi-phase fluids that are vital to energy technologies on a global scale. Fundamental investigations of the complex fluids using advanced research tools would lead to not only better understanding of the multi-scale, multi-phase phenomena (for example, connecting molecular scale interfacial properties to rheology, and rheology to process-scale fluid mechanics), but also enable control of properties of importance in many applications.

### What is the impact on other disciplines?

Other disciplines that would be impacted include oil-gas production and processing in petroleum engineering, energy conversion and thermal energy storage, refrigeration and HVAC (Heating, Ventilation and Air Conditioning), mineral and materials processing, pharmaceutical science, food engineering, data mining, image processing, and high performance computing.

### What is the impact on the development of human resources?

This project has provided opportunities for research, teaching and mentoring in science and engineering fields. It has had a significant impact on the development of human resources expanding the diversity of researchers in the targeted scientific areas of complex fluids research. Among the twelve PhD students and two Master's students supported by the project during the year, seven are women and two of them are from underrepresented minority groups. Two undergraduate students were provided with international research internships in Norway and France. In addition, this PIRE project has enabled training of one postdoctoral researcher and one high school student. All of these researchers have been able to gain advanced knowledge and research skills in experimental, theoretical and/or numerical simulation work. In addition, two Master's students have been able to develop their skills in database and website development. A major goal of this PIRE project at City College of New York is to ensure that adequate partnerships are occurring with international collaborators both at the faculty and student level.

### What is the impact on physical resources that form infrastructure?

Many analytical instruments available in the Grove School of Engineering at CCNY such as a variable temperature Rheometer, X-ray radiography system, gamma densitometer system, a dispersion analyzer (Lumisizer) have been extensively used in this PIRE project. A hot roller was purchased to enable synthesis of model drilling fluids.



### **What is the impact on institutional resources that form infrastructure?**

At the CUNY Advanced Science Research Center (ASRC), NMR and MRI facilities are being used by PIRE researchers to investigate molecular-scale phenomena in PCM Nanoemulsions. The Cryo-SEM system available at Albert Einstein College through the City University of New York (CUNY) School of Public Health was also used to study the microstructures of drilling fluids. Thus, institutional resources available from CUNY have been effectively utilized in this PIRE project, and the user fees paid to the above institutions have contributed to the continuation of their operations.

### **What is the impact on information resources that form infrastructure?**

We purchased a new computer server and software which have been used to perform numerical simulations and serve as a database platform. This computer system has contributed to advancing the research and performing calculations and simulations to answer the project's most pressing research questions. From the beginning of this project, and especially after the campus buildings were shut down due to a COVID-19 pandemic, remote meeting services (BlueJeans and Zoom) made available by City College of New York have been fully utilized in Research Thrust meetings and PIRE Center Management Team meetings.

### **What is the impact on technology transfer?**

A link has been established with a commercial supplier of drilling fluids (MI Swaco) which has provided both knowledge and industrial samples to the PIRE researchers. New technologies developed based on the research conducted with the industrial samples will be transferred back to the oil and gas industry.

Technologies developed based on advances in understanding and control of asphaltene, gas hydrates and PCM Nanoemulsions will be transferred back to the oil/gas, refrigeration and HVAC industries, among others, contributing to the energy efficiency and environmental sustainability.

### **What is the impact on society beyond science and technology?**

An important societal outcome of this project is that it would advance and transform key engineering technologies which are highly relevant to the energy and other industries as well as an important factor in environmental sustainability.

The institutional impacts will result from the international partnerships with some of the most respected international researchers and institutions in the field for generating transformative outcomes that advance and enhance the knowledge needed to further address scientific and economic questions of global significance.

This project has also contributed to STEM education of exceptional undergraduate and graduate students from underrepresented groups by providing them with outstanding research opportunities and extensive international experiences at City College of New York and in partner countries (France, Norway and Germany).

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## **Changes/Problems**

### **Changes in approach and reason for change**

No basic changes in the approach have been made.

### **Actual or Anticipated problems or delays and actions or plans to resolve them**

The City College of New York campus was shut down in mid-March due to a COVID-19 pandemic. Our collaborators' laboratories in France, Norway and Germany were also shut down, so a PhD internship was terminated prematurely in March, 2020, shortly after one of our students arrived at NTNU/SINTEF in Trondheim, Norway. The impact of COVID-19 pandemic on the PIRE project at City College of New York is described in our response to the questionnaire received from NSF on COVID-19 Fall Out attached as Appendix 2.

### **Changes that have a significant impact on expenditures**

Nothing to Report.

### **Significant changes in use or care of human subjects**

Not applicable.

**Significant changes in use or care of vertebrate animals**

Not applicable.

**Significant changes in use or care of biohazards**

Not applicable.

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**Special Requirements**

**Responses to any special reporting requirements specified in the award terms and conditions, as well as any award specific reporting requirements.**

Nothing to report.