Hydrocarbon Reservoirs and Production: Thermodynamics and Rheology

A comprehensive course

By

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Course will be Conducted in Room SB35, Shriram, Chemical Engineering Department, Stanford University

Scope

This five-day course offers a unified framework from classical, molecular and statistical thermodynamics, and molecular simulations to investigate bulk phases, interfaces, and thin films. Rheology of bulk and interfaces is an integral part of the intensive course. The focus of the topics will be on structure in bulk phase, adsorption at the fluid-solid and fluid-fluid interfaces, wettability, viscosification and fracturing, and interfacial rheology. Many topics are covered in relation to efficient hydrocarbon energy production and environmental stewardship. Molecular structure in fluid phases and at the interface and molecular engineering of functional molecules are covered to emphasize the advances that can lead to efficient processes in hydrocarbon energy production. The context of presentations is shale light oil and gas reservoirs, low salinity water injection, improved oil recovery from fluid-fluid interface elasticity, flow assurance in relation to asphaltenes, waxes, and hydrates and use of low concentration of functional molecules, CO_2 fracking, and CO_2 viscosification (in relation to mobility control in CO_2 injection and sequestration and CO_2 fracking). Various structures in bulk phases from micelles and emulsions in hydrocarbon production are included in the course. We will also cover efficient and robust phase behavior computations in relation to CO_2 and light hydrocarbons, and CO. and heavy crude oils. Past climate changes are covered to the level that computations can be performed. The course will go beyond nano-particles; at the atomic scale the vast opportunities that functional molecules can offer for process improvement, efficiency, and safety will be explored. Efficient molecular dissolution of asphaltenes, and colloidal stabilization will be discussed in detail. The vast opportunities that functional molecules at some 100 ppm concentration offer for improved hydrocarbon recovery and production will be a unique feature of this intensive course. The need for combining molecular simulations and molecular thermodynamics will be demonstrated in prediction of molecular structure and adsorption at the fluid-solid interfaces. The concepts will be presented through cartoons to facilitate understanding of a broad range of topics. All presentations and discussions will be based on materials (book, papers, and prepared write-ups) that will be available to participants.

Items of discussion in the course include:

- Unique properties of CO_2 in comparison to nitrogen and methane and other fluids in relation to improved oil recovery in fractured and unfractured reservoirs containing light, heavy, and super-heavy oils. Field experiences from different parts of the world will be discussed.
- Mechanisms of low salinity water injection and effect of salinity and different types of salts on wettability, dissolution, and in micellization and microemulsion
- Why a chemical which gives a recovery in excess of 95% for water injection in the lab may fail in field applications.
- Shale-gas and shale-light oil reservoirs and unique features of shale rocks
- Phase behavior of mixtures of bitumen and various gases and normal alkanes and why normal alkane injection in heavy oils may encounter challenges.
- Strength of cubic-plus-association EOS for a variety of complex problems in aqueous mixtures and asphaltene precipitation
- Predictive capability of EOS and reservoir fluid characterization
- CO_2 mixing with reservoir fluids; Modeling of diffusion flux in reservoir simulators based on chemical potential driving forces
- Asphaltene and resin molecular structure and interaction with water and viscosity reduction
- Formation of nano-particles of asphaltenes and hydrates, and advantage of surface property changes to bulk phase property changes
- Why adsorption measurements at high pressure (say by gravimetric methods) do not provide relevant data and should be combined with molecular simulations to interpret the instrument measurements. Why shale swells from the contact with hydrocarbons and CO_2.
- Why flow in shale nano-pores is by diffusions. Why flow in nano-pores is one to three orders of magnitude higher than the calculations based on the models in the current literature.
- Effect of size of nano-particles on melting and on saturation pressure
- Efficient two- and three-phase split computations

- The link between irreversible thermodynamics and complex diffusion processes and past climate change modeling
- Asphaltene removal from pipes and from rocks by efficient molecular dissolution
- Species distribution in hydrocarbon reservoirs from irreversible thermodynamics
- Hydrate particle stabilization and advancing hydrate flow assurance by small amounts of functionalized molecules
- Basic-level understanding of microemulsion and micellization and application to a variety of problems in hydrocarbon energy production.
- Interfacial Rheology
- Interfacial rheology measurement interpretation in relation to improved oil recovery
- New IOR by increase in interfacial elasticity.
- Thermodynamics of fracking in rocks. Phase field method

Schedule

The course will begin at 8:30 a.m. on June 22 and will end at 6;00 p.m. on June 26. Daily sessions will be from 8:30 a.m. to 4:30 p.m. with a lunch break from 12:15 p.m. to 1:30 p.m. Part of the afternoon sessions will be devoted to discussions.

General course agenda

Day 1

8:30 a.m. – 9:15 a.m.

- Overview of molecular structures in petroleum fluids and fluid-fluid and fluid-solid systems and use of knowledge, modeling, and modern techniques from thermodynamics and rheology in efficient oil and gas production and stewardship of the environment.
- Use of thermodynamic principles in the study of shale gas, shale-light oil, flow assurance, and improved oil recovery
- Use of functional molecules to drastic change of properties
- Property change with size in the nm range

9:15 a.m. – 10:30 a.m.

- Brief review of bulk phase equilibrium thermodynamics
- Removal of fluids from a container and observation of pressure increase!

10:30 a.m. – 10:45 a.m.

- Coffee break

10:45 a.m. – 12:15 p.m.

- General theory of bulk-phase equilibrium thermodynamics in relation to gravity and interfacial effects
- How we increase or decrease normal boiling by the size of the confinement and type of fluids?
- Why condensation and vaporization can be drastically different in single components and in multicomponents? Sometimes the opposite of each other!

12:15 p.m. – 1:30 p.m.

- Lunch break

1:30 p.m. – 2:30 p.m.

- Phase behavior and volumetric description of fluids and fluid mixtures and petroleum fluids from cubic equations of state (EOS)
- Nature of delay and kinetics in various processes including vaporization, condensation, crystallization, and melting
- Why kinetics of vaporization is so different from condensation: the same is true in crystallization and melting
- Why the PR-EOS works so well for reservoir fluids

2:30 p.m. – 3:15 p.m.

- Concept of molecular association
- Phase behavior of water and water-CO_2 mixtures by the cubic-plus-association (CPA) EOS
- Phase behavior in asphaltene precipitation by CPA-EOS

3:15 p.m. – 3:30 p.m.

- Coffee break

3:30 p.m. – 4:30 p.m.

- Phase behavior of bitumen with CO_2 and normal alkanes by CPA-EOS and PR-EOS
- Characterization of reservoir fluids for modeling of various processes, including equilibria of vapor-liquid, vapor-liquid-liquid, wax precipitation, and asphaltene precipitation
- Discussions

Day 2

8:30 a.m. –10:30 a.m.

- Stability and criticality concepts and criteria, and applications in problems of hydrocarbon reservoirs and production; Gibbs free energy surface analysis; How rugged is Gibbs free energy surface? Tangent plane distance analysis
- Two- and three-phase split computations; Stability testing; How to perform phase-split computations with any number of phases with large number of components.
- Brief presentation on phase behavior calculations in UNV space and major difference with the PTVN space.

10:30 a.m. – 10:45 a.m.

- Coffee break

10:45 a.m. – 12:15 p.m.

- General theory of irreversible thermodynamics; Fickian, thermal, and pressure diffusion flux expressions; How can oil float on top of lighter gas forever! Example is Yufutsu field in Japan. This is possible through thermal effects.
- Species distribution in hydrocarbon reservoirs; Past climate changes from irreversible thermodynamics

12:15 p.m. – 1:30 p.m.

- Lunch break

1:30 p.m. – 3:15 p.m.

- Interfacial thermodynamics. Gibbs adsorption equation. New phase formation and driving force. Induction time. Line tension. Effect of size o contact angle. Bubble nucleation. Induction time.

3:15 p.m. – 3:30 p.m.

- Coffee break

3:30 p.m. – 4:30 pm

- Effect of charge of charge on equilibrium in bubbles and droplets.
- Discussions

Day 3

8:30 a.m. – 9:15 a.m.

- Solution-gas drive in permeable media
- Thermodynamics of thin liquid films. Thin film description.
- Effect of size on melting point due to thin films

9:30 a.m. – 10:30 a.m.

- Introduction to micellization and emulsion
- Thermodynamics of micellization and microemulsion; Effect of different salts; Why different salt molecules are so different in their effectiveness?
- Emulsion flow in porous media. Higher flow rates give lower pressure drops. This makes use of Darcy's law inappropriate! Detrimental effect of water-in-oil emulsion in oil recovery.
- Thermodynamics of adsorption in fluid solid interfaces.

10:30 a.m.-10:45 am

- Coffee Break

10:45 a.m.-11:45 am

- The class will be introduced to the science of rheology, which concerns the flow and deformation of complex, non-Newtonian liquids. This subject, which links together fluid mechanics and material science, has great application in the recovery of oil from porous media, wax and hydrate flow assurance, drilling operations that employ complex muds, the design of fracturing fluids, and the stability of oil-water emulsions. Introduction to rheology, the stress tensor in flowing liquids and the rate of strain tensor. Definition of rheological material functions (viscosity, normal stress differences, compliance, dynamic moduli). Shear rheometry and constitutive models.

11:45 a.m. – 12:15 p.m.

- Linear viscoelasticity

12:15 p.m. – 1:30 p.m.

- Lunch break

1:30 p.m. – 2:30 p.m.

- Application of rotational shear rheometry to fluids in the production of oil
- Extensional rheometry. The extensional viscosity of mobile liquids. The design of extensional rheometers and their application to liquids used in enhanced oil recovery.

2:30 p.m. – 3:15 p.m.

- Interfacial rheology. Classification of complex fluid interfaces. Interfacial rheological material functions.

3:15 p.m. – 3:30 p.m.

- Coffee break

3:30 p.m.-4:30 pm

Application of bulk and interfacial rheology to problems in oil production and manufacturing

Day 4

8:30 a.m.-9:30. a.m.

- Asphaltene colloidal stabilization in petroleum fluids by functional molecules; Molecular dissolution of asphaltenes in petroleum fluids at very low concentration of functional molecules; Dissolution of deposited asphaltene molecules back into petroleum fluids
- Effect of water and brine on asphaltene precipitation and deposition and mitigation

9:30 a.m.-10:00 a.m.

- Wax mitigation by crystal modifiers and dispersant. Effect of water

10:00 a.m.-10:15 am

- Coffee Break

10:15 a.m. –11:00 a.m.

- Natural gas hydrates
- Driving force in hydrate formation
- Hydrate anti-agglomeration; Hydrate slurry and hydrate powder by functionalized molecules at low concentrations

11:00 a.m.-12:00 pm

- Low salinity water injection; Mechanisms;
- Improved oil recovery by effective functional molecules at 100 ppm concentration through increase in interface elasticity

12:10 p.m. – 1:30 p.m.

- Lunch break

1:30 p.m.- 2:30 pm

- Introduction to shale-gas and shale-light oil reservoirs
- Condensation and vaporization in nano-pores more than 10 nm
- Phase behavior in shale nano-pores more than 10 nm
- Adsorption and desorption in shale and kerogen media. Swelling from hydrocarbons in kerogen media

2:30 p.m. – 3:30 p.m.

- Statistical thermodynamics; Molecular simulations

3:00 p.m. – 3:15 p.m.

- Coffee break

3:15 p.m. – 4:30 p.m.

- Statistical thermodynamics; Mesoscopic simulations (dissipative particle dynamics, DPD)
- Discussions
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Day 5

8:30 a.m-10:00 a.m.

Adsorption and desorption and swelling in shale: experiments and molecular simulations. Adsorbed phase density from MD simulations

- Why use of EOS with adjusted T_C and P_C should be avoided in phase behavior in shale small nano-pores?

10:00 a.m.–10:15 a.m.

- Coffee break

. 10:15 a.m.–11:15 a.m.
- Flow and Separation of species in shale nano-pores. Flow in shale media.
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11:15 a.m.–12:15 p.m.
- Introduction to thermodynamics of solids. Thermodynamics of fracking and phase field method.

12:15 p.m. – 1:30 p.m.
- Lunch break

1:30 p.m.- 2:15 p.m.
- CO_2 fracking; and CO_2 viscosification by functional molecules

2:15-3:15
- MD simulation of hydrates and hydrate anti-agglomeration; Effect of salt and hydrocarbons on hydrate anti-agglomeration;
- Effect of droplet size on contact angle. MD simulations of contact angle

3:15 pm.- 3:30 pm
- Coffee Break

3:30 pm-4:30 pm
- Discussions and review of the course

4:45 pm-6:00 pm

Hands on Phase Behavior Calculations in 2-Phase and in 3-Phase.

Fees and Registration The fee for attendance is US $2,900. For the staff members of those companies who are members of the Institute, the fee is US $2,300. The course fee includes a copy of the 2015 book, Thermodynamics and Applications in Hydrocarbon Energy and Production, and a file containing relevant write-ups and papers.

Payments should be made by wire transfer or check before April 15, 2020. Please make checks payable to Reservoir Engineering Research Institute and mail your payment to RERI | 595 Lytton Avenue, Suite 2B | Palo Alto, CA 94301. To arrange a payment by a wire transfer, please email us at info@rerinst.org. Payments may be refunded upon cancellation at least 30 days prior to the beginning of the course.

We ask prospective participants to register by completing our online registration form. A block of rooms has been reserved for course participants in downtown Palo Alto. Registrants can book online here. The course will be held at the Department of Chemical Engineering at Stanford University; room SB35 in Shriram.

Hotel Reservation

Hotel booking link.