جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
Science and Technology

Course Syllabus: Thermodynamics of Subsurface Reservoirs - ErSE 209

Division	Physical Science and Engineering Division
Course Number	ErSE 209
Course Title	Thermodynamics of Subsurface Reservoirs
Academic Semester	Spring
Academic Year	2018/2019
Semester Start Date	01/27/2019
Semester End Date	05/23/2019
Class Schedule (Days & Time)	09:00 AM - 10:30 AM | Sun Tue

Instructor(s)

Name	Email	Phone	Office Location	Office Hours
Shuyu Sun	shuyu.sun@kaust.edu.sa	+966128080242	Office 4417, Floor 4, Bldg 1, 1, Al-Khawarizmi (bldg. 1)	3:00-4:30pm Mondays (no appointment needed during office hours)

Teaching Assistant(s)

Name	Email

Course Information

Comprehensive Course Description	Understanding and modeling of subsurface reservoirs in geological formation are required for making decisions associated with the management of the reservoirs. Subsurface reservoirs are complex systems that involve a number of overlapping phenomena, making their simulation a real challenge. Fluid flow and species transport in reservoirs[1] depend strongly on the properties of fluid mixture. As a result, it is important that students get familiar with equilibrium properties and phase behaviors of reservoir fluids under various geological and operating conditions. For example, crude oil is a complex mixture of chemicals that existed for hundred thousands of years and have eventually reached the state of thermodynamic equilibrium. Upon exploration and production, the state of equilibrium that these fluids enjoyed for thousands of years are continuously changed, which leads to changed composition, phase, partition between phases, etc. Understanding these processes requires that students master thermodynamics from the perspective of petroleum reservoirs. This course covers the fundamental laws of thermodynamics and their applications to subsurface reservoirs especially to hydrocarbon reservoirs. Bulk-phase equilibrium thermodynamics is a focus of this course, which prepares students the required thermodynamic skill for compositional petroleum reservoir simulation. Cubic equations of state and their strengths are discussed for pure components and mixtures. In particular, Peng-Robinson equation of state and its modeling parameters are addressed. Detailed calculation procedures are given to predict volumetric properties, gas and liquid phase compositions, thermal properties and sonic velocities of reservoir fluids. Algorithms on flash calculation and stability analysis are considered. We study bisection and successive substitution techniques based on the Rachford-Rice equation as well as Newton's method. Optional advanced topics in this course include 1) prediction of interfacial (surface) tension using EOS, 2) statistical thermodynamics and molecular simulation for phase behaviors of fluids, 3) nonequilibrium and irreversible thermodynamics, especially as applied to reservoir grading, and 4) interfacial thermodynamics and its application to micro-pores and nano-particles for oil reservoirs. [1] The modeling and simulation of flow and transport are covered in separate courses.

Course Description from Program Guide	This course covers the fundamental laws of thermodynamics and their applications to subsurface reservoirs especially to hydrocarbon reservoirs. Bulk phase equilibrium thermodynamics is a focus of this course, which prepares students the required thermodynamic skill for compositional petroleum reservoir simulation. Cubic equations of state and their strengths are discussed for pure components and mixtures. In particular, Peng-Robinson equation of state and its modelling parameters are addressed. Detailed calculation procedures are given to predict volumetric properties, gas and liquid phase compositions, thermal properties and sonic velocities of reservoir fluids. Algorithms on flash calculation and stability analysis are considered. We study bisection and successive substitution techniques based on the Rachford-Rice equation as well as Newtons method. Optional advanced topicsin this course include 1) statistical thermodynamics and molecular simulation for phase behaviors of fluids, 2) nonequilibrium and irreversible thermodynamics, especially as applied to reservoir grading, and 3) interfacial thermodynamics and its application to micro-pores and nano-particles for oil reservoirs.
Goals and Objectives	This course aims at introducing the basic thermodynamics theory and computational techniques modeling the equilibrium properties of subsurface reservoirs, especially petroleum reservoirs. By the end of the course, students should be able to construct EOS (equation of state) models that compute various thermodynamic properties of fluid mixture under various subsurface reservoir conditions. Using a high-level programming language such as MATLAB or R, students are expected to be able to implement the EOS models into numerical simulators that predict equilibrium properties and phase behaviors of subsurface reservoirs.
Required Knowledge	Basic knowledge in engineering thermodynamics and basic programming skills in MATLAB or R, or consent of instructor.
Reference Texts	**Text:** *Thermodynamics and Applications of Hydrocarbons Energy Production*, by Abbas Firoozabadi, published by McGraw-Hill Education; 1 edition (September 16, 2015). ISBN: 978-0071843256. **References:** 1) *Understanding Molecular Simulation: From Algorithms to Applications*, by Daan Frenkel and Berend Smit, published by Academic Press; 2 edition (November 7, 2001). ISBN: 978-0122673511. 2) *Computational Methods for Multiphase Flows in Porous Media* (Computational Science and Engineering), by Zhangxin Chen. Published by Society for Industrial and Applied Mathematics. 1st edition (March 30, 2006). ISBN: 978-0898716061.
Method of evaluation	**30.00**% - Course Project(s) **20.00**% - Quiz(zes) **20.00**% - Midterm exam **20.00**% - Homework /Assignments **10.00**% - Active participation
Nature of the assignments	Nature of the assignments: 1) Active participation: to pay attention to the lecture, usually indicated by asking relevant questions and answering quetions correctly. 2) Pop quizzes: to give in certain classes without notice in advance, usually last 15 minutes. 3) Home assignments: about eight homework sets in total, most of them containing programming exercise. 4) Mid-Term exam: mostly concept recall and formula derivation, but also has problems of simple calculation. 5) Semester project: including presentation and final report. The semester project must have substantial programming content. * The letter grades will be assigned according to: *A*: 95–100; *A-*: 90–94; *B+*: 85–89; *B*: 80–84; *B-*: 75–79; *C+*: 70–74; *C*: 65–69; C-: 60–64; *D+*: 55–59; *D*: 50–54; *D-*: 45–49; *F*: 0–44. * In borderline cases, the instructor reserves the right to subjectively determine grades based on class attendance, class participation, quality of work, etc.
Course Policies	**Attendance:** Regular and punctual attendance is necessary for each student to maximize his/her understanding of the material. Students are expected to wait 15 minutes before leaving if the instructor is not present at the scheduled start time of the class. Excused absences include official university business and personal emergencies (medical, legal, death in the family, etc). It is the student's responsibility to contact the instructor prior to the absence (when possible) and provide the documentation required for excused absences. It is the student's responsibility to make up any deficiency resulting from class absence in a timely manner, including getting class notes (from other students) and assignments. Please carefully read the university attendance policy for additional specifics. **Students who have more than 3 unexcused absences are subject to being dropped from the course.** **Academic Integrity:** As members of the KAUST community, we have a mutual commitment to truthfulness, honor, and responsibility, without which we cannot earn the trust and respect of others. Furthermore, we recognize that academic dishonesty detracts from the value of a KAUST degree. Therefore, we shall not tolerate lying, cheating, or stealing in any form.
Additional Information	

Tentative Course Schedule *(Time, topic/emphasis & resources)*		
Week	**Lectures**	**Topic**
1	Sun 01/27/2019	Motivation & outline of this course; math preparation of thermodynamics (I)
1	Tue 01/29/2019	math preparation of thermodynamics (II)
2	Sun 02/03/2019	Fundamental laws of thermodynamics & applications (I)
2	Tue 02/05/2019	Fundamental laws of thermodynamics & applications (II) HW#1
3	Sun 02/10/2019	Maxwell's relations; Entropy maximum principle;
3	Tue 02/12/2019	Application of Entropy maximum principle; Gibbs-Duhem equation HW#2
4	Sun 02/17/2019	Chemical potentials
4	Tue 02/19/2019	fugacity and fugacity coefficients; HW#3
5	Sun 02/24/2019	Van der Waals Equation of State: derivation
5	Tue 02/26/2019	Van der Waals Equation of State: applications; HW#4
6	Sun 03/03/2019	Peng-Robinson Equation of State: derivation
6	Tue 03/05/2019	Peng-Robinson Equation of State: applications; HW#5
7	Sun 03/10/2019	Calculation of bubble points for fluid mixture
7	Tue 03/12/2019	Calculation of dew points for fluid mixture; HW#6
8	Sun 03/17/2019	Phase stability analysis (I)
8	Tue 03/19/2019	Phase stability analysis (II); HW#7
9	Sun 03/24/2019	[Spring break at KAUST. No class]
9	Tue 03/26/2019	[Spring break at KAUST. No class]
10	Sun 03/31/2019	Flash calculation: Substitutive iteration
10	Tue 04/02/2019	Flash calculation: Newton's method; HW#8
11	Sun 04/07/2019	Review on the thermodynamics of hydrocarbon fluid mixture
11	Tue 04/09/2019	In-Class Mid-Term Examination
12	Sun 04/14/2019	Gradient theory for modeling interfacial tension between phases (I)
12	Tue 04/16/2019	Gradient theory for modeling interfacial tension between phases (II); Term Project Starts
13	Sun 04/21/2019	Monte Carlo molecular simulation techniques and applications (I)
13	Tue 04/23/2019	Monte Carlo molecular simulation techniques and applications (II)
14	Sun 04/28/2019	Molecular dynamics simulation techniques and applications (I)
14	Tue 04/30/2019	Molecular dynamics simulation techniques and applications (II)
15	Sun 05/05/2019	Non-equilibrium/irreversible thermodynamics (I)
15	Tue 05/07/2019	Non-equilibrium/irreversible thermodynamics (II)
16	Sun 05/12/2019	Diffuse interface models for pore-scale compositional multiphase flow (I)
16	Tue 05/14/2019	Diffuse interface models for pore-scale compositional multiphase flow (II)
17	Sun 05/19/2019	Final Exam Week: Term Project Presentation by students; Discussion
17	Tue 05/21/2019	Final Exam Week: Term Project Presentation by students (continued); Discussion

Note

The instructor reserves the right to make changes to this syllabus as necessary.