COURSE ID SHEET

Course No.	5182	NTUA

Semester:	8,10	Core		Elective		Specialization	X

Title: **ADVANCED THERMODYNAMICS**

Aim: The aim of the course is to familiarize students with advanced Chemical Engineering Thermodynamics and its applications. Also, this course aims to provide the students an in-depth analysis of complex phase and chemical equilibrium problems faced in chemical engineering applications, as well as advanced thermodynamic tools. Finally, examples are given where thermodynamics is used to solve basic problems in other engineering disciplines.

Content:

- Thermodynamic equilibrium criteria - Equilibrium in multiphase multi-reaction systems – Phase stability in thermodynamic systems.
- Accurate prediction of vapor pressure with cubic equations of State (EoS)- Accurate prediction of volumetric behavior with cubic EoS - Non-cubic SAFT-type equations – Application of non-cubic EoS to strongly polar mixtures / The CPA EoS.
- Development of advanced mixing rules for cubic EoS - The mathematical approach – The EoS/GE models - Prediction of phase equilibrium with EoS/GE models.
- Liquid-Liquid phase equilibrium formulation - Types of binary phase diagrams - Types of ternary phase diagrams - Liquid-Liquid equilibrium calculations - Formulation of three-phase Vapor-Liquid-Liquid equilibrium - Calculations of three-phase Vapor-Liquid- Liquid equilibrium.
- Formulation of solid-liquid phase equilibrium - Formulation of solid-gas phase equilibrium - Solid-liquid equilibrium calculations - Solid-gas equilibrium calculations. Applications in supercritical extraction technology.
- Classification of reservoir fluids - Reservoir fluid properties - Phase diagrams - Volumetric behavior - Phase equilibrium calculations - Volumetric behavior calculations - Thermodynamic tools for simulating natural gas processes.
- Uses of thermodynamics in biochemical engineering - Equilibrium constant calculations of biochemical reactions - Equilibrium conversion calculations - Calculation of solubility of biomolecules in water and organic solvents - Calculation of distribution coefficients of biomolecules in biphasic systems.
- Applications of thermodynamics in environmental engineering - Prediction of thermodynamic properties for environmental applications (activity coefficients at infinite dilution, vapor pressure of organic pollutants, partition coefficients in the biphasic system 1-octanol/water, solubility of organic pollutants in water, Henry constants). Prediction of the distribution of organic pollutants in the environment - Bioaccumulation of organic pollutants.

Textbook: S. Sandler, Chemical, Biochemical, and Engineering Thermodynamics, 5th Edition, Wiley, 2017.

Hours per semester:									
	LECTURES	**24**	EXERCISES	-	LABORA-TORY	**16**	HOME-WORK	**135**	**TOTAL HOURS: 175**

Student performance/ evaluation:	The evaluation of the students will be done through: • A Final (written) Examination (FE), and • Laboratory Exercises (LE) **The Final Grade results as follows: Final Grade = 0.5 x (FE) + 0.5 x (LE)**