



# THERMODYNAMICS OF FLUID PHASE EQUILIBRIA

## PROF. JAYANT K. SINGH

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**INTENDED AUDIENCE** : Any interested Learners

**PRE-REQUISITES** : An introduction course on Thermodynamics

**INDUSTRIES APPLICABLE TO** : All engineering based industry

### COURSE OUTLINE :

The goal of this course to introduce molecular thermodynamics as a practical tool for engineering applications. In particular, the course would present the first year graduate student or senior undergraduate student a broad introduction to the thermodynamics of phase equilibria typically encountered in designing chemical products and processes. The course is suitable for those students who have completed their course in undergraduate thermodynamics. It would be further useful if the student has also done the first undergraduate course on chemical engineering thermodynamics.

### ABOUT INSTRUCTOR :

Prof. Jayant K. Singh received his B.Tech from IIT Kanpur in chemical engineering in 1997. He subsequently completed his Masters degree in computer science and engineering and Ph.D. in chemical engineering in the area of molecular simulation from SUNY Buffalo, USA in 2004. Dr. Singh is currently a professor in the department of chemical engineering at IIT Kanpur. Dr. Singhs current research interest is in thermodynamics and statistical mechanics, material modeling, confined fluids and development of molecular simulation tools. Dr Singh has co-authored more than 100 peer reviewed articles in international journals of repute. He is a recipient of prestigious awards such as Humboldt Fellow for experienced researcher, Young Engineers of Indian National Academy of Engineers, Amar-Dye Chem award and BRNS Young Scientist Award. He is also an elected member of National Academy of Sciences, Allahabad.

### COURSE PLAN :

**Week 1** : Introduction, Review of first Law for closed and open systems, Properties of ideal gas and real fluids

**Week 2** : Thermodynamics calculus, thermodynamics derivatives, Euler's theorem for homogeneous functions, Legendre's transformations, Derivative in terms of measurable properties, elementary statistical mechanics

**Week 3** : Thermodynamics of Phase Equilibria, Open systems, Ideal Mixtures, Equilibrium in a Heterogeneous Closed System, Fugacity

**Week 4** : Thermodynamic Properties from Volumetric Data, Thermodynamic Properties with P, T as Independent Variable, Fugacity of Liquids and Solids, Thermodynamic Properties with V, T as Independent Variables, Approaches to Phase Equilibria Calculations

**Week 5** : Intermolecular forces, corresponding states, Osmotic systems

**Week 6** : Fugacity in Gas Mixture, Virial equation of state, fugacities from Virial equation, Fugacities at high densities, Solubilities of solids and liquids in compressed gases

**Week 7** : Fugacities in Liquid Mixture: Excess function

**Week 8** : Fugacities in Liquid Mixture: Models and Theory of Solution