

Modelling Phase Equilibria

*Thermodynamic Background
and Practical Tools*

Stanisław Malanowski
Andrzej Anderko

Wiley Series in Chemical Engineering

Modelling Phase Equilibria

Alan Hinchliffe



Modelling Phase Equilibria:

Modelling Phase Equilibria Stanislaw Malanowski, Andrzej Anderko, 1992-05-29 Presents a rigorous development of thermodynamic laws of phase equilibria beginning with fundamental principles accompanied by a short description of the mathematics vital to a clear understanding of basic concepts as well as the practical methods used to calculate phase equilibria Offers excellent explanations of well established thermodynamic tools and novel state of the art techniques representing real fluid behavior Models covered are relevant to the modeling of nonelectrolyte mixtures over wide ranges of pressure temperature composition and molecular diversity *Molecular Thermodynamics of Fluid-Phase Equilibria* John M. Prausnitz, Rudiger N. Lichtenthaler, Edmundo Gomes de Azevedo, 1998-10-22 The classic guide to mixtures completely updated with new models theories examples and data Efficient separation operations and many other chemical processes depend upon a thorough understanding of the properties of gaseous and liquid mixtures *Molecular Thermodynamics of Fluid Phase Equilibria* Third Edition is a systematic practical guide to interpreting correlating and predicting thermodynamic properties used in mixture related phase equilibrium calculations Completely updated this edition reflects the growing maturity of techniques grounded in applied statistical thermodynamics and molecular simulation while relying on classical thermodynamics molecular physics and physical chemistry wherever these fields offer superior solutions Detailed new coverage includes Techniques for improving separation processes and making them more environmentally friendly Theoretical concepts enabling the description and interpretation of solution properties New models notably the lattice fluid and statistical associated fluid theories Polymer solutions including gas polymer equilibria polymer blends membranes and gels Electrolyte solutions including semi empirical models for solutions containing salts or volatile electrolytes Coverage also includes fundamentals of classical thermodynamics of phase equilibria thermodynamic properties from volumetric data intermolecular forces fugacities in gas and liquid mixtures solubilities of gases and solids in liquids high pressure phase equilibria virial coefficients for quantum gases and much more Throughout *Molecular Thermodynamics of Fluid Phase Equilibria* strikes a perfect balance between empirical techniques and theory and is replete with useful examples and experimental data More than ever it is the essential resource for engineers chemists and other professionals working with mixtures and related processes *Molecular Thermodynamics of Fluid Phase Equilibrium* Mr. Rohit Manglik, 2024-01-25 EduGorilla Publication is a trusted name in the education sector committed to empowering learners with high quality study materials and resources Specializing in competitive exams and academic support EduGorilla provides comprehensive and well structured content tailored to meet the needs of students across various streams and levels **Phase Equilibrium Engineering** Esteban Brignole, Selva Pereda, 2013-04-02 In this chapter the problem of sustainability of the chemical and pharmaceutical industries and the principles of green chemistry are outlined In particular the need for secure and environmentally safe solvents ESSs is pointed out There are several ESS alternatives under study nowadays like ionic liquids

polymeric solvents and simple liquids like fatty esters however an increasing attention is being paid to supercritical fluids SCFs for a wide variety of applications in the chemical and pharmaceutical as well as in the materials and electronic industry In the present chapter after an introduction to the fundamentals of SCF extraction PEE principles are applied to several case studies of SCF substrate mixtures of natural products with different types of phase behavior Finally the application of SCF for supercritical micronization is reviewed and a case study is presented

Flash Computation and EoS Modelling for Compositional Thermal Simulation of Flow in Porous Media Duncan Paterson, 2019-02-14 This book investigates a wide range of phase equilibrium modelling and calculation problems for compositional thermal simulation Further it provides an effective solution for multiphase isenthalpic flash under the classical framework and it also presents a new flash calculation framework for multiphase systems which can handle phase equilibrium and chemical reaction equilibrium simultaneously The framework is particularly suitable for systems with many phases and reactions In this book the author shows how the new framework can be generalised for different flash specifications and different independent variables Since the flash calculation is at the heart of various types of compositional simulation the findings presented here will promote the combination of phase equilibrium and chemical equilibrium calculations in future simulators aiming at improving their robustness and efficiency

Phase Equilibrium Engineering Esteban Alberto Brignole, Selva Pereda, 2013-04-02 Traditionally the teaching of phase equilibria emphasizes the relationships between the thermodynamic variables of each phase in equilibrium rather than its engineering applications This book changes the focus from the use of thermodynamics relationships to compute phase equilibria to the design and control of the phase conditions that a process needs Phase Equilibrium Engineering presents a systematic study and application of phase equilibrium tools to the development of chemical processes The thermodynamic modeling of mixtures for process development synthesis simulation design and optimization is analyzed The relation between the mixture molecular properties the selection of the thermodynamic model and the process technology that could be applied are discussed A classification of mixtures separation process thermodynamic models and technologies is presented to guide the engineer in the world of separation processes The phase condition required for a given reacting system is studied at subcritical and supercritical conditions The four cardinal points of phase equilibrium engineering are the chemical plant or process the laboratory the modeling of phase equilibria and the simulator The harmonization of all these components to obtain a better design or operation is the ultimate goal of phase equilibrium engineering Methodologies are discussed using relevant industrial examples The molecular nature and composition of the process mixture is given a key role in process decisions Phase equilibrium diagrams are used as a drawing board for process implementation

Models for Thermodynamic and Phase Equilibria Calculations Stanley I. Sandler, 1993-10-07 Provides a definitive state of the art review of the models used in applied thermodynamics Discusses all aspects of thermodynamic modeling relevant to the chemical industry including activity coefficient models equations of state

mixture group contribution methods and specialized procedures for polymer and electrolyte solutions

Phase Equilibria in Ionic Liquid Facilitated Liquid-Liquid Extractions Anand Bharti, Debashis Kundu, Dharamashi Rabari, Tamal Banerjee, 2017-03-31 This book provides a comprehensive overview of ionic liquid based separation techniques. The glimpse of thermodynamic predictive models along with global optimization techniques will help readers understand the separation techniques at molecular and macroscopic levels. Experimental and characterization techniques are coupled with model based predictions so as to provide multicomponent data for the scientific community. The models will focus more on the a priori based predictions which gives higher emphasis on hydrogen bonded systems. Particle Swarm Optimization (PSO) technique will also eventually help the readers to apply optimization technique to an extraction process. The overriding goal of this work is to provide pathways for leading engineers and researchers toward a clear understanding and firm grasp of the phase equilibria of Ionic Liquid systems.

Foundations of Molecular Modeling and Simulation Edward J. Maginn, Jeffrey Errington, 2021-03-25 This highly informative and carefully presented book comprises select proceedings of Foundation for Molecular Modelling and Simulation (FOMMS) 2018. The contents are written by invited speakers centered on the theme Innovation for Complex Systems. It showcases new developments and applications of computational quantum chemistry, statistical mechanics, molecular simulation, and theory, and continuum and engineering process simulation. This volume will serve as a useful reference to researchers, academicians, and practitioners alike.

Chemical Modelling Alan Hinchliffe, 2007-10-31 Chemical Modelling: Applications and Theory comprises critical literature reviews of molecular modelling, both theoretical and applied. Molecular modelling in this context refers to modelling the structure, properties, and reactions of atoms, molecules, materials. Each chapter is compiled by experts in their fields and provides a selective review of recent literature incorporating sufficient historical perspective for the non-specialist to gain an understanding. With chemical modelling covering such a wide range of subjects, this Specialist Periodical Report serves as the first port of call to any chemist, biochemist, materials scientist, or molecular physicist needing to acquaint themselves with major developments in the area.

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