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J.Richard Elliott, Carl T. Lira

Chapter 18: Electrolyte Solutions 693. 18.1

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Student Supplements - J.Richard Elliott, Carl T. Lira

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Supplementary Materials for Students

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J. Richard Elliott is Professor of Chemical Engineering at the University of Akron in Ohio. He has taught courses ranging from freshman tools to senior process design as well as thermodynamics at every level. He has worked with the NIST lab in Boulder and ChemStations in Houston. He holds a Ph.D. from Pennsylvania State University.

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Learning objectives, problem-solving strategies for energy balances and phase equilibria, chapter summaries, and “important equations” for every chapter Extensive practical examples, especially coverage of non-ideal mixtures, which include water contamination via hydrocarbons, polymer blending/recycling, oxygenated fuels, hydrogen bonding, osmotic pressure, electrolyte solutions, zwitterions and biological molecules, and other contemporary issues Supporting software in formats for both MATLAB® and spreadsheets Online supplemental sections and resources including instructor slides, ConcepTests, coursecast videos, and other useful resources

This book consists of a number of papers regarding the thermodynamics and structure of multicomponent systems that we have published during the last decade. Even though they involve different topics and different systems, they have something in common which can be considered as the “signature” of the present book. First, these papers are concerned with “difficult” or very nonideal systems, i. e. systems with very strong interactions (e. g. , hydrogen bonding) between components or systems with large differences in the partial molar volumes of the components (e. g. , the aqueous solutions of proteins), or systems that are far from “normal” conditions (e. g. , critical or near-critical mixtures). Second, the conventional thermodynamic methods are not sufficient for the accurate treatment of these mixtures. Last but not least, these systems are of interest for the pharmaceutical, biomedical, and related industries. In order to meet the thermodynamic



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challenges involved in these complex mixtures, we employed a variety of traditional methods but also new methods, such as the fluctuation theory of Kirkwood and Buff and ab initio quantum mechanical techniques. The Kirkwood-Buff (KB) theory is a rigorous formalism which is free of any of the approximations usually used in the thermodynamic treatment of multicomponent systems. This theory appears to be very fruitful when applied to the above mentioned “difficult” systems.

The selection of the most adequate thermodynamic model in a process simulation is an issue that most process engineer has to face sooner or later. This book, conceived as a practical guide, aims at providing adequate answers by analysing the questions to be looked at. The analysis (first chapter) yields three keys that are further discussed in three different chapters. (1) A good understanding of the properties required in the process, and their method of calculation is the first key. The second chapter provides to that end in a synthetic manner the most important equations that are derived from the fundamental principles of thermodynamics. (2) An adequate description of the mixture, which is a combination of models and parameters, is the second key. The third chapter makes the link between components and models, both from a numerical (parameterisation) and physical (molecular interactions) point of view. Finally, (3) a correct view of the phase behaviour and trends in regard of the process conditions is the third key. The fourth chapter illustrates the phase behaviour and makes model recommendations for the most significant industrial

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systems. A decision tree is provided at the end of this chapter. In the last chapter, the key questions are reviewed for a number of typical processes. This book is intended for process engineers, who are not specialists of thermodynamics but are confronted with this kind of problems and need a reference book, as well as process engineering students who will find an original approach to thermodynamics, complementary of traditional lectures

This title aims to teach how to invent optimal and sustainable chemical processes by making use of systematic conceptual methods and computer simulation techniques. The material covers five sections: process simulation; thermodynamic methods; process synthesis; process integration; and design project including case studies. It is primarily intended as a teaching support for undergraduate and postgraduate students following various process design courses and projects, but will also be of great value to professional engineers interested in the newest design methods. Provides an introduction to the newest design methods. Of great value to undergraduate and postgraduate students as well as professional engineers. Numerous examples illustrate theoretical principles and design issues.

Using an applications perspective Thermodynamic Models for Industrial Applications provides a unified framework for the development of various

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thermodynamic models, ranging from the classical models to some of the most advanced ones. Among these are the Cubic Plus Association Equation of State (CPA EoS) and the Perturbed Chain Statistical Association Fluid Theory (PC-SAFT). These two advanced models are already in widespread use in industry and academia, especially within the oil and gas, chemical and polymer industries. Presenting both classical models such as the Cubic Equations of State and more advanced models such as the CPA, this book provides the critical starting point for choosing the most appropriate calculation method for accurate process simulations. Written by two of the developers of these models, *Thermodynamic Models for Industrial Applications* emphasizes model selection and model development and includes a useful “which model for which application” guide. It also covers industrial requirements as well as discusses the challenges of thermodynamics in the 21st Century.

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