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Chapter 14, Interpretation of reaction energy balance from other texts in terms of the notation in Elliott and Lira Chemical Reaction Engineering, 3rd ed., Levenspiel, 1999. Elements of Chemical Reaction Engineering, 3rd ed., Fogler, 1999.

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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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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. , hydgen bonding) between components or systems with large differences in

the partial molar v- umes 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 th- modynamic 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 ind- tries. In order to meet the thermodynamic challenges involved in these complex mixtures, we employed a variety of traditional methods but also new methods, such as the fluctuation t- ory 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 - proximations usually used in the thermodynamic treatment of multicomponent systems. This theory appears to be very fruitful when applied to the above mentioned “ difficult ” systems.

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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 principes 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

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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

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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

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also covers industrial requirements as well as discusses the challenges of thermodynamics in the 21st Century.

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