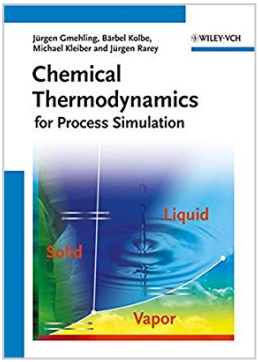

Chemical Thermodynamics for Process Simulation

By J?rgen Gmehling, B?rbel Kolbe, Michael Kleiber, J?rgen Rarey

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This is the only book to apply thermodynamics to real-world process engineering problems, explaining the thermodynamics behind simulations from the view of academic and industrial authors to users of simulation programs. It comprises numerous solved examples, which simplify the understanding of the often complex calculation procedures, and discusses their advantages and disadvantages. The text also includes such special models as for formaldehyde, polymers, and associating compounds. Estimation methods for thermophysical properties and phase equilibria and thermodynamics of alternative separation processes are covered, as are new developments from recent years.

For a deeper understanding additional problems are given at the end of each chapter. To solve the complex problems prepared Mathcad files, Excel files or the DDBSP Explorer version can be accessed via the Internet.

While written for an advanced level, the text is easy to understand for every chemical engineer and chemist with a basic education in thermodynamics and phase equilibria, teaching students the engineering perspective of thermodynamics but also of interest to all companies active in chemistry, pharmacy, oil and gas processing, petrochemistry, refinery, food production, environmental protection and engineering.

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Editorial Review

Review
"The authors of this excellent book on chemical thermodynamics have achieved something rare taking one of the dreariest theoretical sciences and making
it accessible.
This book is a treasure trove of fundamental thermodynamic knowledge with the guidance necessary to apply the theory to practical applications.
The first eight chapters deal primarily with thermodynamic concepts, such as pure component behaviour (Chapter 1). properties of mixtures (Chapter 2), phase equilibria and solid state equilibria (Chapters 4 and 8). In each of these chapters the authors manage to breakdown thermodynamics into its essential building blocks and guide the reader through the increasing complexity. This is a good refresher for those who studied thermodynamics as a student or a good introduction to those being exposed to thermodynamics for the first time.
However, be warned. This is not the basics of thermodynamics: the reader quickly gets amongst the mathematics - but it is present in a direct and concise manner that anyone familiar with undergraduate mathematics will be able to comprehend.
Though the title has 'for process simulations, most of the thermodynamic discussion is on the fundamental Level, with only the later parts of each chapter progressing into simulation models. Examples are equations of state for fluid system phase equilibria (Chapter-1) and the NRTL model in electrolyte solutions (Chapter 7). This distinction makes Chemical thermodynamics for process simulations a great general reference source.
The worked examples hit the Goldilocks zone for problems - not too easy, not too hard - and this reviewer found them to successfully illustrate the various topics.
The second half of the book focuses more on the applied side ? applying thermodynamic theory to membrane processes (Chapter 9) and polymers (Chapter 10), as well as to reactions and equilibriums (Chapter 12). Here, the reader can become confused if not well versed in the topics of interest, since some prior knowledge is assumed.
The final chapter is not really a chapter, but rather an invitation for readers to download thermodynamic and process examples from the internet to be applied in software programs such as Mathcad. This is a great example of broadening the education value through technology, and should be copied bymore authors.
If you are interested in detailed and accessible thermodynamics, start and finish with this book."
- Chemistry in Australia, September 2012

From the Back Cover
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About the Author
J?rgen Gmehling studied chemical engineering in Essen and chemistry at the University of Dortmund, where he gained his doctorate in inorganic chemistry in 1973. From 1977-1978 he worked with Prof. J.M. Prausnitz at the Department of Chemical Engineering in Berkeley, California, before taking up his present post as Professor of Chemical Engineering at the University of Oldenburg in 1989. He is also president and CEO of DDBST GmbH, Oldenburg, as well as cofounder of LTP GmbH, part of the Carl von Ossietzky University of Oldenburg. Professor Gmehling has received various awards, such as the Arnold-Eucken Prize from the GVC, the Rossini Lecture Award 2008 from the International Association of Chemical Thermodynamics, and the Gmelin-Beilstein Denkm?nze from the GDCh. His research is concentrated on the computer-aided synthesis, design and optimization of chemical processes.

After graduating in chemical engineering, B?rbel Kolbe completed her thesis in 1983 at the University of Dortmund in the research group led by J?rgen Gmehling, with whom she continued to work for another three years. During this time she participated in the publication of the Dechema Chemistry Data Series on VLE as well as the first edition of this book in German. Dr. Kolbe has been working for over twenty years as a senior process engineer first for Krupp Koppers GmbH and, since 1997, for ThyssenKrupp Uhde. The main focus of her research is on thermophysical properties, thermal separation technology and new processes.

After graduating in mechanical engineering, Michael Kleiber worked as a scientific assistant at the TU Brunswick, where he completed his thesis in 1994. After this, he worked for the former Hoechst AG and its successors in the fields of process development, process simulation and engineering calculations, before moving to ThyssenKrupp Uhde as a Chief Development Engineer. Dr. Kleiber is a member of the German Board of Thermodynamics and contributor to several standard works on process engineering, such as the VDI Heat Atlas, Winnacker-K?chler and Ullmann's Encyclopedia of Industrial Chemistry.

J?rgen Rarey studied chemistry and gained his PhD in chemical engineering. He has held a permanent position at the University of Oldenburg in Prof. Gmehling's group since 1989, the same year he cofounded DDBST GmbH. For the past 20 years he has taught many courses on applied thermodynamics for chemical process simulation for external participants from industry both in Oldenburg, as well as in-house for companies from around the world. Dr. Rarey is also an honorary professor in Durban, South Africa.

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