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The Thermodynamics of Phase and Reaction Equilibria Wiley

"This book approaches the subject of material and energy balances from two directions. First, it emphasizes the fundamental principles of the conservation of mass and energy, and the consequences of these two principles. Second it applies the techniques of computational chemistry to materials processing, and introduces new software developed by the author especially for material and heat balances. The third edition reflects the changes in the professional engineer's practice in the last 30 years, reflecting the dramatic shift away from metallurgical engineering and the extractive industry towards

materials engineering. A large and growing number of recent graduates are employed in such fields as semiconductor processing, environmental engineering, and the production and processing of advanced and exotic materials for aerospace, electronic and structural applications. The advance in computing power and software for the desktop computer has significantly changed the way engineers make computations, and the biggest change comes from the computational approach used to solve problems. The spreadsheet program Excel is used extensively throughout the text as the main computational "engine" for solving material and energy balance equations, and for statistical analysis of data. The use of Excel and the introduction of the add-in programs enables the study of a range of variables on critical process parameters, and emphasis is placed on multi-device flowsheets with recycle, bypass, and purge streams whose material and heat balance equations were previously too complicated to solve by the normally-used hand calculator. The Excel-based program FlowBal helps the user set up material and heat balance equations for processes with multiple streams and units"--
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The field of Chemical Engineering and its link to computer science is in constant evolution and new engineers have a variety of tools at their disposal to tackle their everyday problems. Introduction to Software for Chemical Engineers, Second Edition provides a quick guide to the use of various computer packages for chemical engineering applications. It covers a range of software applications from Excel and general mathematical packages such as MATLAB and MathCAD to process simulators, CHEMCAD and ASPEN, equation-based modeling languages, gProms, optimization software such as GAMS and AIMS, and specialized software like CFD or DEM codes. The different packages are introduced and applied to solve typical problems in fluid mechanics, heat and mass transfer, mass and energy balances, unit operations, reactor engineering, process and equipment design and control. This new edition offers a wider view of packages including open source software such as R, Python and Julia. It also includes complete examples in ASPEN Plus, adds ANSYS Fluent to CFD codes, Lingo to the optimization packages, and discusses Engineering Equation Solver. It offers a global idea of the capabilities of the software used in the chemical engineering field and provides examples for solving real-world problems. Written by leading experts, this book is a must-have reference for chemical engineers looking to grow in their careers through the use of new and improving computer software. Its user-friendly approach to simulation and optimization as well as its example-based presentation of the software, makes it a perfect teaching tool for both undergraduate and master levels.