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Introduction to chemical engineering computing / Bruce A. Finlayson. – 2nd ed. p. cm. Includes index. ISBN 978-0-470-93295-7 (pbk.) 1. Chemical engineering–Data processing. I. Title. TP184.F56 2012 660.0285–dc23 2011045242 Printed in the United States of America 10 987654321

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INTRODUCTION TO CHEMICAL ENGINEERING COMPUTING

This pdf illustrates how to use the programming language Python to solve the problems posed in the book Introduction to Chemical Engineering Computing, Bruce A. Finlayson, Wiley

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(2006-2014). The material mirrors the use of MATLAB in the book, and solves the examples in Chapters 2, 3, 4, and 8.

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Introduction to Chemical Engineering Computing teaches professionals and students the kinds of problems they will have to solve, the types of computer programs needed to solve these problems, and...

Step-by-step instructions enable chemical engineers to master key software programs and solve complex problems. Today, both students and professionals in chemical engineering must solve increasingly complex problems dealing with refineries, fuel cells, microreactors, and pharmaceutical plants, to name a few. With this book as their guide, readers learn to solve these problems using their computers and Excel, MATLAB, Aspen Plus, and COMSOL Multiphysics. Moreover, they learn how to check their solutions and validate their results to make sure they have solved the problems correctly. Now in its Second Edition, Introduction to Chemical Engineering Computing is based on the author's firsthand teaching experience. As a result, the emphasis is on problem solving. Simple introductions help readers become conversant with each program and then tackle a broad range of problems in chemical engineering, including: Equations of state Chemical reaction equilibria Mass balances with recycle streams Thermodynamics and simulation of mass transfer equipment Process simulation Fluid flow in two and three dimensions All the chapters contain clear instructions, figures, and examples to guide readers through all the programs and types of chemical engineering problems. Problems at the end of each chapter, ranging from simple to difficult, allow readers to gradually build their skills, whether they solve the problems themselves or

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intteams. In addition, the book ' s accompanying website lists the core principles learned from each problem, both from a chemical engineering and a computational perspective. Covering a broad range of disciplines and problems within chemical engineering, Introduction to Chemical Engineering Computing is recommended for both undergraduate and graduate students as well as practicing engineers who want to know how to choose the right computer software program and tackle almost any chemical engineering problem.

Introduction to Chemical Engineering Analysis Using Mathematica, Second Edition reviews the processes and designs used to manufacture, use, and dispose of chemical products using Mathematica, one of the most powerful mathematical software tools available for symbolic, numerical, and graphical computing. Analysis and computation are explained simultaneously. The book covers the core concepts of chemical engineering, ranging from the conservation of mass and energy to chemical kinetics. The text also shows how to use the latest version of Mathematica, from the basics of writing a few lines of code through developing entire analysis programs. This second edition has been fully revised and updated, and includes analyses of the conservation of energy, whereas the first edition focused on the conservation of mass and ordinary differential equations. Offers a fully revised and updated new edition, extended with conservation of energy Covers a large number of topics in chemical

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engineering analysis, particularly for applications to reaction systems Includes many detailed examples Contains updated and new worked problems at the end of the book Written by a prominent scientist in the field

The field of chemical engineering is undergoing a global “renaissance,” with new processes, equipment, and sources changing literally every day. It is a dynamic, important area of study and the basis for some of the most lucrative and integral fields of science. Introduction to Chemical Engineering offers a comprehensive overview of the concept, principles and applications of chemical engineering. It explains the distinct chemical engineering knowledge which gave rise to a general-purpose technology and broadest engineering field. The book serves as a conduit between college education and the real-world chemical engineering practice. It answers many questions students and young engineers often ask which include: How is what I studied in the classroom being applied in the industrial setting? What steps do I need to take to become a professional chemical engineer? What are the career diversities in chemical engineering and the engineering knowledge required? How is chemical engineering design done in real-world? What are the chemical engineering computer tools and their applications? What are the prospects, present and future challenges of chemical engineering? And so on. It also provides the information new chemical engineering hires would need to excel and cross the critical novice engineer stage of their career. It is expected that this book will enhance students understanding and performance in the field and the development of the profession worldwide. Whether a new-hire engineer or a veteran in the field, this is a must—have volume for any chemical engineer ’ s library.

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A Practical, Up-to-Date Introduction to Applied Thermodynamics, Including Coverage of Process Simulation Models and an Introduction to Biological Systems Introductory Chemical Engineering Thermodynamics, Second Edition, helps readers master the fundamentals of applied thermodynamics as practiced today: with extensive development of molecular perspectives that enables adaptation to fields including biological systems, environmental applications, and nanotechnology. This text is distinctive in making molecular perspectives accessible at the introductory level and connecting properties with practical implications. Features of the second edition include Hierarchical instruction with increasing levels of detail: Content requiring deeper levels of theory is clearly delineated in separate sections and chapters Early introduction to the overall perspective of composite systems like distillation columns, reactive processes, and biological systems 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 concise book is a broad and highly motivational introduction for first-year engineering students to the exciting of field of chemical engineering. The material in the text is meant to

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precede the traditional second-year topics. It provides students with, 1) materials to assist them in deciding whether to major in chemical engineering; and 2) help for future chemical engineering majors to recognize in later courses the connections between advanced topics and relationships to the whole discipline. This text, or portions of it, may be useful for the chemical engineering portion of a broader freshman level introduction to engineering course that examines multiple engineering fields.

While various software packages have become essential for performing unit operations and other kinds of processes in chemical engineering, the fundamental theory and methods of calculation must also be understood to effectively test the validity of these packages and verify the results. *Computer Methods in Chemical Engineering, Second Edition* presents the most used simulation software along with the theory involved. It covers chemical engineering thermodynamics, fluid mechanics, material and energy balances, mass transfer operations, reactor design, and computer applications in chemical engineering. The highly anticipated Second Edition is thoroughly updated to reflect the latest updates in the featured software and has added a focus on real reactors, introduces AVEVA Process Simulation software, and includes new and updated appendixes. Through this book, students will learn the following:

- What chemical engineers do
- The functions and theoretical background of basic chemical engineering unit operations
- How to simulate chemical processes using software packages
- How to size chemical process units manually and with software
- How to fit experimental data
- How to solve linear and nonlinear algebraic equations as well as ordinary differential equations

Along with exercises and references, each chapter contains a theoretical

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description of process units followed by numerous examples that are solved step by step via hand calculation and computer simulation using Hysys/UniSim, PRO/II, Aspen Plus, and SuperPro Designer. Adhering to the Accreditation Board for Engineering and Technology (ABET) criteria, the book gives chemical engineering students and professionals the tools to solve real problems involving thermodynamics and fluid-phase equilibria, fluid flow, material and energy balances, heat exchangers, reactor design, distillation, absorption, and liquid extraction. This new edition includes many examples simulated by recent software packages. In addition, fluid package information is introduced in correlation to the numerical problems in book. An updated solutions manual and PowerPoint slides are also provided in addition to new video guides and UniSim program files.

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

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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.

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