



# Introduction to Chemical Engineering Computing

Bruce A. Finlayson

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**MATLAB Applications in Chemical Engineering** Chyi-Tsong Chen, 2022-05-20 This book addresses the applications of MATLAB and Simulink in the solution of chemical engineering problems By classifying the problems into seven different categories the author organizes this book as follows Chapter One Solution of a System of Linear Equations Chapter Two Solution of Nonlinear Equations Chapter Three Interpolation Differentiation and Integration Chapter Four Numerical Solution of Ordinary Differential Equations Chapter Five Numerical solution of Partial Differential Equations Chapter Six Process Optimization Chapter Seven Parameter Estimation Each chapter is arranged in four major parts In the first part the basic problem patterns that can be solved with MATLAB are presented The second part describes how to apply MATLAB commands to solve the formulated problems in the field of chemical engineering In the third and the fourth parts exercises and summary of MATLAB instructions are provided

respectively The description of the chemical engineering example follows the sequence of problem formulation model analysis MATLAB program design execution results and discussion In this way learners are first aware of the basic problem patterns and the underlying chemical engineering principles followed by further familiarizing themselves with the relevant MATLAB instructions and programming skills Readers are encouraged to do exercises to practice their problem solving skills and deepen the fundamental knowledge of chemical engineering and relevant application problems The table of contents is listed below Chapter 1 Solution of a System of Linear Equations 1 1 1 Properties of linear equation systems and the relevant MATLAB commands 1 1 2 Chemical engineering examples 10 1 3 Exercises 43 1 4 Summary of the MATLAB commands related to this chapter 48 Chapter 2 Solution of Nonlinear Equations 51 2 1 Relevant MATLAB commands and the Simulink solution interface 51 2 2 Chemical engineering examples 70 2 3 Exercises 103 2 4 Summary of MATLAB commands related to this chapter 122 Chapter 3 Interpolation Differentiation and Integration 125 3 1 Interpolation commands in MATLAB 125 3 2 Numerical differentiation 131 3 3 Numerical integration 153 3 4 Chemical engineering examples 157 3 5 Exercises 183 3 6 Summary of the MATLAB commands related to this chapter 195 Chapter 4 Numerical Solution of Ordinary Differential Equations 197 4 1 Initial value problems for ordinary differential equations 197 4 2 Higher order ordinary differential equations 222 4 3 Stiff differential equations 227 4 4 Differential algebraic equation system 232 4 5 Boundary valued ordinary differential equations 236 4 6 Chemical engineering examples 254 4 7 Exercises 285 4 8 Summary of the MATLAB commands related to this chapter 308 Chapter 5 Numerical Solution of Partial Differential Equations 311 5 1 Classifications of PDEs 311 5 2 The MATLAB PDE toolbox 316 5 3 Chemical engineering examples 341 5 4 Exercises 388 5 5 Summary of the MATLAB commands related to this chapter 397 Chapter 6 Process Optimization 399 6 1 The optimization problem and the relevant MATLAB commands 399 6 2 Chemical engineering examples 448 6 3 Exercises 481 6 4 Summary of the MATLAB commands related to this chapter 501 Chapter 7 Parameter Estimation 503 7 1 Parameter estimation using the least squares method 503 7 2 Chemical engineering examples 517 7 3 Exercises 549 7 4 Summary of the MATLAB commands related to this chapter 560 References 563 Index 569

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Wissenschaftliches Rechnen whoever has to be blamed for that scientists from outside the field have been confused about the some what strange distinction between scientific and non scientific computations And the insiders i e those who are at least convinced of always comput ing in a very scientific way are far from being happy with this summary of their daily work even if further characterizations like High Performance or Engineering try to make things clearer usually with very modest suc cess however Moreover to increase the unfortunate confusion of terms who knows the differences between Computational Science and Engineering as indicated in the title of the series these proceedings were given the honour to be published in and Scientific and Engineering Computing as chosen for the title of our book Actually though the protagonists of scientific com puting persist in its independence as a scientific discipline and rightly so of course the ideas behind the term diverge wildly Consequently the variety of answers one can get to the question What is scientific computing is really impressive and ranges from the serious nothing else but numerical analysis up to the more mocking consuming as much CPU time as possible on the most powerful number crunchers accessible

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Parallel and Distributed Scientific and Engineering Computing Yi Pan, Laurence Tianruo Yang, 2004 In the not too distant future every researcher and professional in science and engineering fields will have to understand parallel and distributed computing With hyperthreading in Intel processors hypertransport links in AMD processors multi core silicon in today's high end microprocessors from IBM and emerging cluster and grid computing parallel and distributed computers have moved into the mainstream of computing To fully exploit these advances in computer architectures researchers and professionals must start to design parallel or distributed software systems and algorithms for their scientific and engineering applications Parallel and distributed scientific and engineering computing has become a key technology which will play an important part in determining or at least shaping future research and development activities in many academic and industrial branches This book reports on the recent important advances in the area of parallel and distributed computing for science and engineering applications Included in the book are selected papers from prestigious workshops such as PACT SHPSEC IPDPS PDSECA and ICPP HPSECA together with some invited papers from prominent researchers around the world The book is basically divided into five main sections These chapters not only provide novel ideas new experimental results and hands-on experience in this field but also stimulate the future research activities in the area of parallel and distributed computing for science and engineering applications

High Performance Scientific And Engineering Computing Michael Breuer, Franz Durst, Christoph Zenger, 2012-12-06 In Douglas Adams book Hitchhiker's Guide to the Galaxy hyper intelligent beings reached a point in their existence where they wanted to understand the purpose of their own existence and the universe They built a supercomputer called Deep Thought and upon completion they asked it for the answer to the ultimate question of life the universe and everything else The computer worked for several millennia on the answers to all these questions When the day arrived for hyper intelligent beings to receive the answer they were stunned shocked and disappointed to hear that the answer was simply 42 The still open questions to scientists and engineers are typically much simpler and consequently the answers are more reasonable Furthermore because human beings are too impatient and not ready to wait for such a long period high performance computing techniques have been developed leading to much faster answers Based on these developments in the last two decades scientific and engineering computing has evolved to a key technology which plays an important role in

determining or at least shaping future research and development activities in many branches of industry Development work has been going on all over the world resulting in numerical methods that are now available for simulations that were not foreseeable some years ago However these days the availability of supercomputers with Teraflop performance supports extensive computations with technical relevance A new age of engineering has started      **Reliable Engineering Computing** ,      *The Chemical Engineer* ,2009      *Chemical Engineering Education* ,2003

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