



**IN THE NAME OF ALLAH**  
**MOST GRACIOUS, MOST MERCIFUL**



# INTRODUCTION TO MATHEMATICAL MODELING OF CHEMICAL PROCESSES

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## PREFACE

Many courses in the undergraduate chemical engineering curriculum need, with various degrees of importance, some concepts on modeling. This includes courses such as process design, process control, reaction engineering and numerical methods. The availability of fast computers has also pushed chemical engineers to adopt a more rigorous approach to modeling. This text is a modest contribution to the modeling of chemical processes. It is essentially the compilation of notes used by the three authors in their teaching of various courses in the chemical engineering department, in undergraduate as well as in graduate level. The book is, therefore, designed for undergraduate students as well as first year graduate students. The book is divided into five chapters and two appendices. In the first chapter, we present an overview of modeling together with the classification of systems and models. The purpose is to give the student a big picture of the purpose of modeling, building steps for a model, the fundamental equations and the nature of the resulting model. In the second chapter, the student is introduced to the practical aspects of modeling with the help of various examples that scan macroscopic models. In the third chapter, the student is exposed to various examples of microscopic models. In each example, the emphasis is put on the making of the right assumptions, the choice of the right control volume, the writing of the right balance equations and the analysis of the obtained model. The fourth chapter of this book is devoted to the presentation of the equations of change in various coordinates systems. Based on our experience, it is the building of microscopic models that presents the biggest challenge to the students. But once the equations of change are derived, they can be effective tools in the hand of the student to understand the physical meanings of the terms involved in the equation and to help him make the right simplifications for the model. The fifth chapter covers aspects of empirical modeling with emphasis on linear regression methods. While this book is aimed primarily at introducing basic elements of modeling, the solution of the resulting model equations is obviously the ultimate goal of modeling. We presented an appendix with a very brief introduction of the solution of the various model types encountered in the book. We also included in the appendix some software (FORTRAN and MATLAB) used to solve the various types of model equations. Another appendix was included to present a case study covering aspects of modeling, validation and simulation as applied to an industrial multi-stage flash desalination plant.



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