

Chapter 1

Overview

Great progress is being made in mathematical modeling of chemical and biochemical processes. Advances in computing, transport theory, chemical experimentation, and statistics all contribute to making process modeling more effective. Computerized laboratories are providing more and better data, and progress continues in statistical design and analysis of experiments. Modern computer hardware and software are making more realistic process models tractable, prompting fuller analyses of experimental data to build better models and establish probable process mechanisms.

This book will acquaint the reader with some of the important tools and strategies now available for investigating chemical processes and systems on personal computers. We present some useful mathematical models, numerical methods for solving them, and statistical methods for testing and discriminating candidate models with experimental data. The software package *Athena Visual Studio*, obtained from www.AthenaVisual.com, will enable you to do these computations and view the results on your personal computer screen, print them and transmit them. Familiarity with Microsoft Windows (1998 or later) is required, but little knowledge of Fortran, since Athena converts equation statements directly into Fortran code as described in the Athena tutorial on your computer's desktop.

Appendix A provides an introduction to linear algebra and to matrix methods for solving linear equation systems. A study or review of this appendix will prepare the reader for the applications of this material in Chapters 1 through 7. The other appendices describe Athena's solvers DDAPLUS and GREGPLUS, which are updated versions of our former subroutines DDASAC (Double-Precision Differential-Algebraic Sensitivity Analysis Code) and GREG (Generalized REGression package).

Chapter 2 deals with principles of chemical reaction modeling and gives some model forms for use in later chapters. A strong distinction is maintained between rates of reaction and of species production by defining reaction rates as frequencies of particular reaction events per unit reactor space. Various levels of reactor modeling are considered in Chapter 3 and implemented in Athena's samples of its solvers.

Chapter 4 begins the study of statistical methods and their role in process investigations. Concepts introduced include sample spaces, probability densities and distributions, the central limit theorems of DeMoivre and Lindeberg, the normal distribution, and its extension to multivariate

data. Chapter 5 presents Bayes' theorem and Jeffreys rule for unprejudiced inference of model parameters and auxiliary functions from experimental data.

Chapters 6 and 7 treat statistical aspects of process modeling, including parameter and function estimation, goodness-of-fit testing, model discrimination, and selection of conditions for additional experiments. Chapter 6 focuses on modeling with single-response data, and Chapter 7 deals with modeling with multiresponse data. Our software package GREGPLUS, included in Athena and described in Appendix C, performs these tasks for single or multiple models presented by the user.

Our aim in this book is to present modeling as a way of gaining insight, with or without detailed computations. With this in mind, we describe some diagnostic plots proposed by Yang and Hougen (1950) for reactions with a single controlling step, which give valuable clues for choosing good models and weeding out models that won't work.

Our students and colleagues have found it useful to examine the software descriptions and examples before choosing projects in their fields of interest. We suggest that the reader also begin by examining Appendices A, B, and C to learn the capabilities of Athena's solvers.

REFERENCES and FURTHER READING

Yang, K. H., and O. A. Hougen, Determination of mechanism of catalyzed gaseous reactions. *Chem. Eng. Prog.* **46** (1950).