

Analysis of Enzyme Reaction Kinetics

2-Volume Set

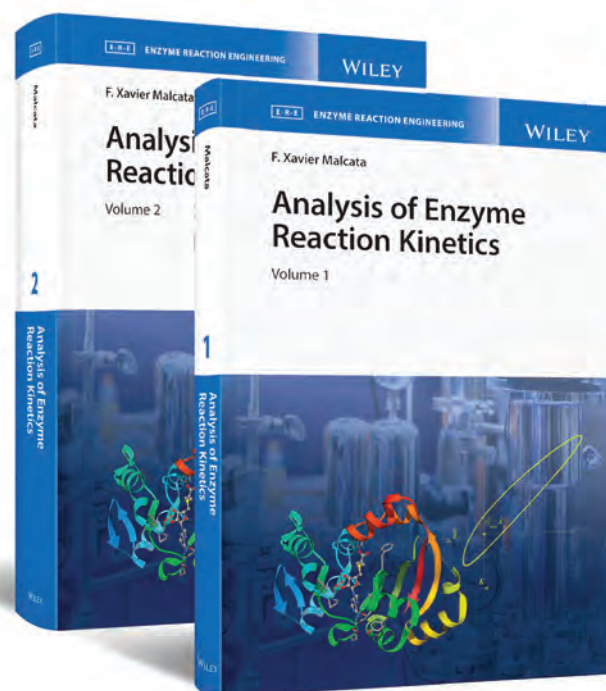
By F. Xavier Malcata

Chemical Engineering

Comprehensively introduces readers to modelling of rate of enzymatic reactions, including effects of physicochemical parameters

Analysis of Enzyme Reaction Kinetics describes rate expressions pertaining to enzymatic reactions, including modulation by physicochemical factors, as well as tools for prediction and control of how fast substrates are transformed to products. Volume 1 details rate expressions mathematically derived from mechanistic postulates and is complemented by appropriate statistical approaches to fit them to experimental data. Volume 2 discusses the effects of physical and chemical parameters upon the rates of both enzyme-catalyzed and enzyme-deactivation reactions.

Starting with basic concepts and historical perspectives, the first volume introduces readers to the mathematics of rate expressions. It then goes on to cover kinetic features and the many forms of Michaelis & Menten's-type rate expressions (single and multiple enzymes, autocatalysis, single and multiple substrates, multiphasic systems, etc.), and concludes with the statistical analysis of rate expressions – including the assessment of data, fitting of models to data, and generation of data themselves. The second volume introduces readers to physicochemical modulation of reaction rate – starting with basic concepts, and looking specifically at temperature-, mechanical force-, pH- and compound-driven effects: both unimodal and bimodal deactivation are considered.



2 Volumes | Print ISBN 9781119490241
Hardcover | 1472 pages | March 2022
List price US\$425.00

Analysis of Enzyme Reaction Kinetics is a comprehensive work for those studying or working with enzyme reactions, or practitioners involved in the control of reactors.



THE AUTHOR

F. Xavier Malcata, PhD, is Full Professor at the Department of Chemical Engineering at the University of Porto in Portugal, and Researcher at LEPABE – Laboratory for Process Engineering, Environment, Biotechnology and Energy. He is the author of more than 400 highly cited journal papers, eleven books, four edited books, and fifty chapters in edited books. He has been awarded the Elmer Marth Educator Award by the International Association of Food Protection (USA) and the William V. Cruess Award for excellence in teaching by the Institute of Food Technologists (USA).



Please contact your local Wiley sales representative to place your orders or for any queries.

WILEY

Analysis of Enzyme Reaction Kinetics

2-Volume Set

TABLE OF CONTENTS

About the Author

Series Preface

Preface

Volume 1

Part 1 Mathematical Approach to Rate Expressions

1. Introduction
 - 1.1. Basic Concepts
 - 1.2. Chemical Mechanism and Rate Expression
 - 1.3. Historical Perspective
 - 1.4. Further Refinements
 - 1.5. Multisubstrate Approaches
 - 1.6. Objective
 - 1.7. Strategy
2. Rate Expression
 - 2.1. Kinetic Features
 - 2.2. Order of Reaction
3. Michaelis and Menten's Rate Expression with Single Enzyme
 - 3.1. Michaelis and Menten's Rationale
 - 3.2. Graphical Interpretation
 - 3.3. Semilogarithmic Plot
 - 3.4. Eisinger and Cornish-Bowden's Plot
 - 3.5. Dixon's Plot
 - 3.6. Concentration of Enzyme Forms
 - 3.7. Best Reparameterization
 - 3.8. van Slyke and Cullen's Rationale
 - 3.9. Briggs and Haldane's Rationale
 - 3.10. Absolute Sensitivity to Lumped Parameters
 - 3.11. Relative Error of Alternative Derivations
 - 3.12. Relative Sensitivity to Intrinsic Parameters
 - 3.13. Biochemical Rationale
 - 3.14. Derivatives of Rate Expression
4. Michaelis and Menten's Rate Expression with Multiple Enzymes
 - 4.1. Several Isozymes
 - 4.2. Two Isozymes
 - 4.3. Infinite Isozymes
5. Michaelis and Menten's Rate Expression with Autocatalysis
6. Michaelis and Menten's Rate Expression with Multiphasic Systems
7. Improved Rate Expression with Single Enzyme
 - 7.1. Morrison's Rationale
 - 7.2. Graphical Interpretation
 - 7.3. Low Enzyme Concentration
 - 7.4. Best Reparameterization
 - 7.5. Kim's Rationale
 - 7.6. Graphical Interpretation
 - 7.7. Specific Kinetic Features
 - 7.8. Absolute Sensitivity to Intrinsic Parameters

- 7.9. Improved Simulation of Initial Transients
- 7.10. Improved Simulation of Final Transient
8. Alternative Forms of Michaelis and Menten's Rate Expression
 - 8.1. Integrated Form
 - 8.2. Linearized Form
9. Rate Expressions for Multisubstrate Reactions
 - 9.1. Shortcut Approaches to Pseudo Steady State
 - 9.2. Uni Uni Mechanism
 - 9.3. Ordered Bi Uni Mechanism
 - 9.4. Other Uni/Bi and Bi/Bi Mechanisms
 - 9.5. Simplification of Multisubstrate Rate Expressions

Part 2 Statistical Approach to Rate Expressions

10. Introduction
 - 10.1. Introductory Concepts
 - 10.2. Objective
 - 10.3. Strategy
11. Assessment of Data and Models
 - 11.1. Independence Checks
 - 11.2. Normality Checks
 - 11.3. Homoskedasticity Checks
 - 11.4. Linearity Checks
 - 11.5. Relationship Checks
 - 11.6. Adequacy Checks
 - 11.7. Sufficiency Checks
12. Fitting of Models to Data
 - 12.1. Linear Regression Analysis
 - 12.2. Improved Regression Analysis
 - 12.3. Nonlinear Regression Analysis
13. Generation of Data
 - 13.1. Empirical Designs
 - 13.2. Mechanistic Designs

Further Reading

Volume 2

Part 3 Physical Modulation of Reaction Rate

14. Introduction
 - 14.1. Basic Concepts
 - 14.2. Thermodynamic Approach
 - 14.3. Kinetic Approach
 - 14.4. Physical Deactivation of Enzymes
 - 14.5. Objective
 - 14.6. Strategy
15. Unimodal Deactivation
 - 15.1. Simple Reversible Deactivation
 - 15.2. Simple Irreversible Deactivation
 - 15.3. General Deactivation
16. Bimodal Deactivation
 - 16.1. Simple Reversible Deactivation
 - 16.2. Simple Irreversible Deactivation

17. Effects upon Nonelementary Reactions
18. Temperature-Driven Modulation
 - 18.1. Thermodynamic Formulation of Temperature Dependence of Elementary Steps
 - 18.2. Kinetic Formulation of Temperature Dependence of Elementary Steps
 - 18.3. Improvement of Parameter Fitting
19. Mechanical Force-Driven Modulation
 - 19.1. Normal Elastic Forces
 - 19.2. Tangential Elastic Forces
 - 19.3. Tangential Plastic Forces
20. Response of Enzyme Deactivation
21. Response of Enzymatic Reaction

Part 4 Chemical Modulation of Reaction Rate

22. Introduction
 - 22.1. Basic Concepts
 - 22.2. Thermodynamic Approach
 - 22.3. Kinetic Approach
 - 22.4. Chemical Deactivation
 - 22.5. Chemical Modulation
 - 22.6. Objective
 - 22.7. Strategy
23. pH-Driven Modulation
 - 23.1. Proteolysis of Enzyme Only
 - 23.2. Proteolysis of Enzyme and Substrate
24. Ionic Strength-Driven Modulation
25. pH-Driven Deactivation
 - 25.1. Reversible Decay
 - 25.2. Irreversible Decay
26. Self-Deactivation
27. Microbial Deactivation
28. Heterologous Bimodal Deactivation
 - 28.1. Reversible Deactivation
 - 28.2. Irreversible Deactivation
29. Heterologous Unimodal Deactivation
 - 29.1. Reversible Deactivation
 - 29.2. Irreversible Deactivation
30. Mechanism Discrimination
 - 30.1. Sequential Random Bi Bi
 - 30.2. Sequential Ordered Bi Bi
 - 30.3. Ping Pong Bi Bi
 - 30.4. Graphical Comparison
31. Homologous Modulation 1227
 - 31.1. Independent Sites
 - 31.2. Sequential Transition
 - 31.3. Concerted Transition
 - 31.4. Asymptotic Patterns

Further Reading

Index

Mathematics for Enzyme Reaction Kinetics and Reactor Performance

2-Volume Set

By F. Xavier Malcata

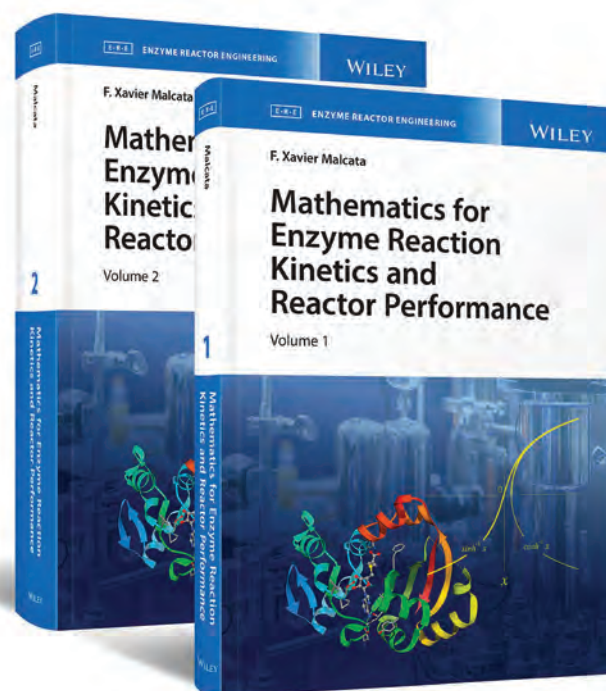
Chemical Engineering

This two volume set details the mathematical background required for systematic and rational simulation of both enzyme reaction kinetics and enzyme reactor performance

Mathematics for Enzyme Reaction Kinetics and Reactor Performance is the first set in a unique multi-volume collection on Enzyme Reactor Engineering, and relates specifically to the wide mathematical background required for systematic and rational simulation of both reaction kinetics and reactor performance; and to fully understand and capitalize on the modelling concepts developed. It accordingly reviews basic and useful concepts of Algebra (first volume), and Calculus and Statistics (second volume).

A brief overview of such native algebraic entities as scalars, vectors, matrices and determinants constitutes the starting point of the first volume; the major features of germane functions are then addressed. Vector operations ensue, followed by calculation of determinants. Finally, exact methods for solution of selected algebraic equations—including sets of linear equations, are considered, as well as numerical methods for utilization at large.

The second volume begins with an introduction to basic concepts in calculus, i.e. limits, derivatives, integrals and differential equations; limits, along with continuity, are further expanded afterwards, covering uni- and multivariate cases, as well as classical theorems. After recovering the concept of differential and applying it to generate (regular and partial) derivatives, the most important rules of differentiation of functions, in explicit, implicit and parametric form, are retrieved – together with the nuclear theorems supporting simpler manipulation thereof. Next, the book touches on the methods of solution of differential equations for practical applications, followed by analytical geometry and vector calculus.



2 Volumes | Print ISBN 9781119490289
Hardcover | 1072 pages | April 2020
List price US\$350.00

Mathematics for Enzyme Reaction Kinetics and Reactor Performance is an excellent reference book for students in the fields of chemical, biological and biochemical engineering, and will appeal to all those interested in the fascinating area of white biotechnology.



THE AUTHOR

F. Xavier Malcata, PhD, is Full Professor at the Department of Chemical Engineering at the University of Porto in Portugal, and Researcher at LEPABE – Laboratory for Process Engineering, Environment, Biotechnology and Energy. He is the author of more than 400 highly cited journal papers, eleven books, four edited books, and fifty chapters in edited books. He has been awarded the Elmer Marth Educator Award by the International Association of Food Protection (USA) and the William V. Cruess Award for excellence in teaching by the Institute of Food Technologists (USA).



Please contact your local Wiley sales representative to place your orders or for any queries.

WILEY

Mathematics for Enzyme Reaction Kinetics and Reactor Performance

2-Volume Set

TABLE OF CONTENTS

About the Author

Series Preface

Preface

Volume 1

Part 1 Basic Concepts of Algebra

1. Scalars, Vectors, Matrices, and Determinants

2. Function Features

2.1. Series

2.2. Multiplication and Division of Polynomials

2.3. Trigonometric Functions

2.4. Hyperbolic Functions

3. Vector Operations

3.1. Addition of Vectors

3.2. Multiplication of Scalar by Vector

3.3. Scalar Multiplication of Vectors

3.4. Vector Multiplication of Vectors

4. Matrix Operations

4.1. Addition of Matrices

4.2. Multiplication of Scalar by Matrix

4.3. Multiplication of Matrices

4.4. Transposal of Matrices

4.5. Inversion of Matrices

4.6. Combined Features

5. Tensor Operations

6. Determinants

6.1. Definition

6.2. Calculation

6.3. Eigenvalues and Eigenvectors

7. Solution of Algebraic Equations

7.1. Linear Systems of Equations

7.2. Quadratic Equation

7.3. Lambert's W Function

7.4. Numerical Approaches

Further Reading

Volume 2

Part 2 Basic Concepts of Calculus

8. Limits, Derivatives, Integrals, and Differential Equations

9. Limits and Continuity

9.1. Univariate Limit

9.2. Multivariate Limit

9.3. Basic Theorems on Limits

9.4. Definition of Continuity

9.5. Basic Theorems on Continuity

10. Differentials, Derivatives, and Partial Derivatives

10.1. Differential

10.2. Derivative

10.3. Dependence Between Functions

10.4. Optimization of Univariate Continuous Functions

10.5. Optimization of Multivariate Continuous Functions

11. Integrals

11.1. Univariate Integral

11.2. Multivariate Integral

11.3. Optimization of Single Integral

11.4. Optimization of Set of Derivatives

12. Infinite Series and Integrals

12.1. Definition and Criteria of Convergence

12.2. Taylor's Series

12.3. Gamma Function and Factorial

13. Analytical Geometry

13.1. Straight Line

13.2. Simple Polygons

13.3. Conical Curves

13.4. Length of Line

13.5. Curvature of Line

13.6. Area of Plane Surface

13.7. Outer Area of Revolution Solid

13.8. Volume of Revolution Solid

14. Transforms

14.1. Laplace's Transform

14.2. Legendre's Transform

15. Solution of Differential Equations

15.1. Ordinary Differential Equations

15.2. Partial Differential Equations

16. Vector Calculus

16.1. Rectangular Coordinates

16.2. Cylindrical Coordinates

16.3. Spherical Coordinates

16.4. Curvature of Three-dimensional Surfaces

16.5. Three-dimensional Integration

17. Numerical Approaches to Integration

17.1. Calculation of Definite Integrals

17.2. Integration of Differential Equations

Part 3 Basic Concepts of Statistics

18. Continuous Probability Functions

18.1. Basic Statistical Descriptors

18.2. Normal Distribution

18.3. Other Relevant Distributions

19. Statistical Hypothesis Testing

20. Linear Regression

20.1. Parameter Fitting

20.2. Residual Characterization

20.3. Parameter Inference

20.4. Unbiased Estimation

20.5. Prediction Inference

20.6. Multivariate Correction

Further Reading