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Nota di contenuto	Computer-Aided Modeling of Reactive Systems; Contents; Chapter 1. Overview; REFERENCES and FURTHER READING; Chapter 2. Chemical Reaction Models; 2.1 STOICHIOMETRY OF REACTION SCHEMES; 2.2 COMPUTABILITY OF REACTION RATES FROM DATA; 2.3 EQUILIBRIA OF CHEMICAL REACTIONS; 2.4 KINETICS OF ELEMENTARY STEPS; 2.5 PROPERTIES OF REACTION NETWORKS; 2.6 EVIDENCE FOR REACTION STEPS; PROBLEMS; REFERENCES and FURTHER READING; Chapter 3. Chemical Reactor Models; 3.1 MACROSCOPIC CONSERVATION EQUATIONS; 3.1.1 Material Balances; 3.1.2 Total Energy Balance; 3.1.3 Momentum Balance; 3.1.4 Mechanical Energy Balance 3.2 HEAT AND MASS TRANSFER IN FIXED BEDS 3.3 INTERFACIAL STATES IN FIXED-BED REACTORS; 3.4 MATERIAL TRANSPORT IN POROUS CATALYSTS; 3.4.1 Material Transport in a Cylindrical Pore Segment; 3.4.2 Material Transport in a Pore Network; 3.4.3 Working Models of Flow and Diffusion in Isotropic Media; 3.4.4 Discussion; 3.4.5 Transport and Reaction in Porous Catalysts; 3.5 GAS PROPERTIES AT LOW

PRESSURES; 3.6 NOTATION; REFERENCES and FURTHER READING; Chapter 4. Introduction to Probability and Statistics; 4.1 STRATEGY OF DATA-BASED INVESTIGATION; 4.2 BASIC CONCEPTS IN PROBABILITY THEORY
4.3 DISTRIBUTIONS OF SUMS OF RANDOM VARIABLES 4.4 MULTIRESPONSE NORMAL ERROR DISTRIBUTIONS; 4.5 STATISTICAL INFERENCE AND CRITICISM; PROBLEMS; REFERENCES and FURTHER READING; Chapter 5. Introduction to Bayesian Estimation; 5.1 THE THEOREM; 5.2 BAYESIAN ESTIMATION WITH INFORMATIVE PRIORS; 5.3 INTRODUCTION TO NONINFORMATIVE PRIORS; 5.4 JEFFREYS PRIOR FOR ONE-PARAMETER MODELS; 5.5 JEFFREYS PRIOR FOR MULTIPARAMETER MODELS; 5.6 SUMMARY; PROBLEMS; REFERENCES and FURTHER READING; Chapter 6. Process Modeling with Single-Response Data; 6.1 THE OBJECTIVE FUNCTION $S()$
6.2 WEIGHTING AND OBSERVATION FORMS 6.3 PARAMETRIC SENSITIVITIES; NORMAL EQUATIONS; 6.4 CONSTRAINED MINIMIZATION OF $S()$; 6.4.1 The Quadratic Programming Algorithm GRQP; 6.4.2 The Line Search Algorithm GRSI; 6.4.3 Final Expansions Around ; 6.5 TESTING THE RESIDUALS; 6.6 INFERENCES FROM THE POSTERIOR DENSITY; 6.6.1 Inferences for the Parameters; 6.6.2 Inferences for Predicted Functions; 6.6.3 Discrimination of Rival Models by Posterior Probability; 6.7 SEQUENTIAL PLANNING OF EXPERIMENTS; 6.7.1 Planning for Parameter Estimation; 6.7.2 Planning for Auxiliary Function Estimation
6.7.3 Planning for Model Discrimination 6.7.4 Combined Discrimination and Estimation; 6.7.5 Planning for Model Building; 6.8 EXAMPLES; 6.9 SUMMARY; 6.10 NOTATION; PROBLEMS; REFERENCES and FURTHER READING; Chapter 7. Process Modeling with Multiresponse Data; 7.1 PROBLEM TYPES; 7.2 OBJECTIVE FUNCTION; 7.2.1 Selection of Working Responses; 7.2.2 Derivatives of Eqs. (7.2-1) and (7.2-3); 7.2.3 Quadratic Expansions; Normal Equations; 7.3 CONSTRAINED MINIMIZATION OF $s()$; 7.3.1 Final Expansions Around ; 7.4 TESTING THE RESIDUALS; 7.5 POSTERIOR PROBABILITIES AND REGIONS 7.5.1 Inferences Regarding Parameters

Sommario/riassunto

Learn to apply modeling and parameter estimation tools and strategies to chemical processes using your personal computer. This book introduces readers to powerful parameter estimation and computational methods for modeling complex chemical reactions and reaction processes. It presents useful mathematical models, numerical methods for solving them, and statistical methods for testing and discriminating candidate models with experimental data. Topics covered include: Chemical reaction models Chemical reactor models Probability and statistics Bayesian estimation Process modeling with si
