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Nota di contenuto	Contents; Dedication; Preface; Chapter 1. Background of Combinatorial Catalyst Development (M. Baerns); Bibliography; Chapter 2. Approaches in the Development of Heterogeneous Catalysts (M. Baerns); 2.1. Fundamental Aspects; 2.2. High-throughput Technologies for Preparation and Testing in Combinatorial Development of Catalytic Materials; 2.2.1. Selection of Potential Elements for Defining the Multi-parameter Compositional Space of Catalytic Materials; 2.2.2. Experimental Tools for Preparing and Testing Large Numbers of Catalytic-material Specimens; 2.2.2.1. Preparation of catalytic materials 2.2.2.2. Testing and screening of catalytic materialsBibliography; Chapter 3. Mathematical Methods of Searching for Optimal Catalytic Materials (M. Holena); 3.1. Introduction; 3.2. Statistical Design of Experiments; 3.3. Optimisation Methods for Empirical Objective Functions; 3.4. Evolutionary Optimisation: The Main Approach to Seek Optimal Catalysts; 3.4.1. Dealing with Constraints in Genetic Optimisation; 3.5. Other Stochastic Optimisation Methods; 3.6. Deterministic Optimisation; 3.6.1. Utilizability of Methods with Derivatives in Catalysis; Bibliography

Chapter 4. Generating Problem-Tailored Genetic Algorithms for Catalyst Search (M. Holena) 4.1. Using a Program Generator - Why and How; 4.2. Description Language for Optimisation Tasks in Catalysis; 4.3. Tackling Constrained Mixed Optimisation; 4.4. A Prototype Implementation; Bibliography; Chapter 5. Analysis and Mining of Data Collected in Catalytic Experiments (M. Holena); 5.1. Similarity and Difference Between Data Analysis and Mining; 5.2. Survey of Existing Methods; 5.2.1. Statistical Methods; 5.2.2. Extraction of Logical Rules from Data; 5.3. Case Study with the Synthesis of HCN Bibliography Chapter 6. Artificial Neural Networks in the Development of Catalytic Materials (M. Holena); 6.1. What are Artificial Neural Networks?; 6.1.1. Network Architecture; 6.1.2. Important Kinds of Neural Networks; 6.1.3. Activity of Neurons; 6.1.4. What do Neural Networks Compute?; 6.2. Approximation Capability of Neural Networks; 6.3. Training Neural Networks; 6.4. Knowledge Obtainable from a Trained Network; Bibliography; Chapter 7. Tuning Evolutionary Algorithms with Artificial Neural Networks (M. Holena); 7.1. Heuristic Parameters of Genetic Algorithms 7.2. Parameter Tuning Based on Virtual Experiments 7.3. Case Study with the Oxidative Dehydrogenation of Propane; Bibliography; Chapter 8. Improving Neural Network Approximations (M. Holena); 8.1. Importance of Choosing the Right Network Architecture; 8.2. Influence of the Distribution of Training Data; 8.3. Boosting Neural Networks; 8.4. Case Study with HCN Synthesis Continued; Bibliography; Chapter 9. Applications of Combinatorial Catalyst Development and An Outlook on Future Work (M. Baerns); 9.1. Introduction; 9.2. Experimental Applications of Combinatorial Catalyst Development 9.3. Methodology

Sommario/riassunto

The book provides a comprehensive treatment of combinatorial development of heterogeneous catalysts. In particular, two computer-aided approaches that have played a key role in combinatorial catalysis and high-throughput experimentation during the last decade - evolutionary optimization and artificial neural networks - are described. The book is unique in that it describes evolutionary optimization in a broader context of methods of searching for optimal catalytic materials, including statistical design of experiments, as well as presents neural networks in a broader context of data analysis.
