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2.1.11 Experimental Design; 2.1.12 Process Integration; 2.1.13 Process Synthesis; 2.1.14 Data Reconciliation; 2.1.15 Mathematical Computing Software; 2.1.16 Chemometrics; 2.2 Some Observations on the Practical Use of Modelling and Simulation; 2.2.1 Reliability of Models and Simulations; 2.2.2 The Role of Industry as Final User of Modelling and Simulation; 2.2.3 Modelling and Simulation in Innovations; 2.2.4 Role of Modelling in Technology Transfer and Knowledge Management; 2.2.5 Role of the Universities in Modelling and Simulation Development; References

3 Mathematical Modelling Based on Transport Phenomena; 3.1 Algorithm for the Development of a Mathematical Model of a Process; 3.1.1 Some Observations about the Start of the Research; 3.1.2 The Limits of Modelling Based on Transport Phenomena; 3.2 An Example: From a Written Description to a Simulator; 3.3 Chemical Engineering Flow Models; 3.3.1 The Distribution Function and the Fundamental Flow Models; 3.3.2 Combined Flow Models; 3.3.3 The Slip Flow Effect on the Efficiency of a Mechanically Mixed Reactor in a Permanent Regime; 3.3.4 Dispersion Flow Model; 3.3.5 Examples; 3.3.5.1 Mechanically Mixed Reactor for Reactions in Liquid Media; 3.5.2 Gas Flow in a Fluidized Bed Reactor; 3.3.5.3 Flow in a Fixed Bed Catalytic Reactor; 3.3.6 Flow Modelling using Computational Fluid Dynamics; 3.4 Complex Models and Their Simulators; 3.4.1 Problem of Heating in a Zone Refining Process; 3.4.2 Heat Transfer in a Composite Medium; 3.4.3 Fast Chemical Reaction Accompanied by Heat and Mass Transfer; 3.5 Some Aspects of Parameters Identification in Mathematical Modelling; 3.5.1 The Analytical Method for Identifying the Parameters of a Model; 3.5.1.1 The Pore Radius and Tortuosity of a Porous Membrane for Gas Permeation

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#### Sommario/riassunto

A description of the use of computer aided modeling and simulation in the development, integration and optimization of industrial processes. The two authors elucidate the entire procedure step-by-step, from basic mathematical modeling to result interpretation and full-scale process performance analysis. They further demonstrate similitude comparisons of experimental results from different systems as a tool for broadening the applicability of the calculation methods. Throughout, the book adopts a very practical approach, addressing actual problems and projects likely to be encountered by the

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