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Autore	Britz Dieter
Titolo	Digital Simulation in Electrochemistry // by Dieter Britz, Jörg Strutwolf
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ISBN	3-319-30292-2
Edizione	[4th ed. 2016.]
Descrizione fisica	1 online resource (498 p.)
Collana	Monographs in Electrochemistry, , 1865-1836
Disciplina	541.3702854
Soggetti	Electrochemistry Analytical chemistry Chemistry, Physical and theoretical Chemometrics Cheminformatics Analytical Chemistry Theoretical and Computational Chemistry Math. Applications in Chemistry Computer Applications in Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Introduction -- Basic Equations -- Approximations to Derivatives -- Ordinary Differential Equations -- The Explicit Method -- Boundary Conditions -- Arbitrary Intervals -- The Commonly Used Implicit Methods -- Other Methods -- Adsorption -- Uncompensated Resistance and Capacitance -- Two-Dimensional Systems -- Migration -- Convection -- Performance -- Programming -- Simulation Packages -- Appendices: Some Mathematical Proofs -- Useful Procedures -- Example Programs.
Sommario/riassunto	This book explains how the partial differential equations (pdes) in electroanalytical chemistry can be solved numerically. It guides the reader through the topic in a very didactic way, by first introducing and discussing the basic equations along with some model systems as test cases systematically. Then it outlines basic numerical approximations for derivatives and techniques for the numerical solution of ordinary

differential equations. Finally, more complicated methods for approaching the pdes are derived. The authors describe major implicit methods in detail and show how to handle homogeneous chemical reactions, even including coupled and nonlinear cases. On this basis, more advanced techniques are briefly sketched and some of the commercially available programs are discussed. In this way the reader is systematically guided and can learn the tools for approaching his own electrochemical simulation problems. This new fourth edition has been carefully revised, updated and extended compared to the previous edition (Lecture Notes in Physics Vol. 666). It contains new material describing migration effects, as well as arrays of ultramicroelectrodes. It is thus the most comprehensive and didactic introduction to the topic of electrochemical simulation.
