

1. Record Nr.	UNINA9910959309003321
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Titolo	Groundwater contamination : discretization and simulation of systems for convection-diffusion-dispersion reactions // Jurgen Ernst Geiser
Pubbl/distr/stampa	New York, : Nova Science Publishers, c2009
ISBN	1-60876-524-5
Edizione	[1st ed.]
Descrizione fisica	1 online resource (172 p.)
Disciplina	363.739/4
Soggetti	Groundwater - Pollution - Simulation methods Hazardous waste sites - Simulation methods Groundwater - Pollution - Mathematical models Dispersion - Mathematical models Discrete-time systems - Mathematical models Discrete geometry
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 (p. [149]-158) and index.
Nota di contenuto	Intro -- GROUNDWATER CONTAMINATION: DISCRETIZATION AND SIMULATION OF SYSTEMS FOR CONVECTION-DIFFUSION-DISPERSION REACTIONS -- GROUNDWATER CONTAMINATION: DISCRETIZATION AND SIMULATION OF SYSTEMS FOR CONVECTION-DIFFUSION-DISPERSION REACTIONS -- Contents -- Preface -- Introduction -- Modeling -- 2.1. Introduction and Motivation -- 2.2. Physics of the Mathematical Model -- 2.3. Mathematical Model -- Discretization -- 3.1. Introduction -- 3.2. Finite Volume Method -- 3.3. Notations for Finite Volume Method -- 3.4. Discretization of the Convection Equation -- 3.5. Discretization of the Diffusion-Dispersion Equation -- 3.6. Discretization of the Reaction Equation -- 3.7. Discretization of the Convection-Reaction Equation with Embedded Analytical Solutions -- Operator-Splitting Methods -- 4.1. Splitting Method of First Order -- 4.2. Strang Splitting and Methods of Higher Order -- 4.3. Iterative Operator-Splitting Method -- 4.4. Application of the Splitting Methods -- 4.5. LOD and ADI Methods -- 4.6. Nonlinear Splitting Methods -- 4.7. Remarks about the Operator-Splitting Methods -- Analytical Solutions for One-Dimensional Convection-Reaction Equations -- 5.1.

Analytical Solutions for Convection-Reaction Equations with Variable Retardation Factors -- 5.2. Calculating the Analytical Solution of Mass -- Iterative Methods and Multigrid Methods -- 6.1. Introduction -- 6.2. Linear Algebra -- 6.3. Linear Iterative Method -- 6.4. Introduction to Multigrid Methods -- Software Package r3t -- 7.1. Introduction -- 7.2. Rough Structuring of the Software Packages -- 7.3. UG Software Toolbox -- 7.4. Software Package d3f -- 7.5. Software Package r3t -- Model Problems -- 8.1. Introduction for Model Problems -- 8.2. Error Norms and Orders of Convergence to Evaluate Numerical Results -- 8.3. One-Dimensional Model Problems for Linear Equilibrium-Sorption. 8.4. Two-Dimensional Model Problem for Linear Equilibrium-Sorption -- 8.5. Realistic Model for a Potential Damage Event -- Outlook -- 9.1. Conclusion and Outlook -- Appendix A Properties, Transformable Functions, and Partial Fraction Expansion of the Laplace Transformation -- Appendix B General Solutions for Ordinary Differential Equations -- References -- Index.

Sommario/riassunto

This work arose from research results of the interdisciplinary centre for scientific computing at the University of Heidelberg as well as of the Humboldt University. The contribution of this work is the simulation of contaminated ground water developed from models about the disposal of severely contaminated material, i.e. radioactive fuels or chemical waste products. The model is based on equations for convection-diffusion-dispersion reactions. The equation in the present book is used for the modelling of a radionuclide transport of pollutants in ground water as well as for chemical irreversible reactions. While solving such problems, so-called multi-scale processes arise. Conventional treatment of black-box discretisation and solution methods are impossible or complicated. Hence, physically motivated methods are used, i.e. to integrate one-dimensional analytical solutions of convection-reaction equations. Especially so-called decomposition methods were emphasized. These methods decouple the different scales and solve the equations based on scales with each other. Therefore the previous coupling errors between the terms of the equations can be controlled and minimised with iterative methods. Furthermore, analytical solutions could be used for comparisons with the numerical solutions. In this work the theoretical derivations of solutions as well as their application in numerical methods for realistic calculations could be acquired. The methods were assembled in a program package that had been developed in a project to evolve a program for modelling the transport of pollutants in ground water. Some realistic damage events could be calculated based on dates from the partner GRS in Braunschweig, Germany.

2. Record Nr.	UNISALENTO991004409828807536
Titolo	La qualità nelle narrazioni per l'infanzia : sguardi pedagogici su contenuti analogici e digitali rivolti a bambine e bambini / Cosimo Di Bari (a cura di)
Pubbl/distr/stampa	Roma : Anicia, 2024
ISBN	9788867098095
Descrizione fisica	292 p. : ill. ; 24 cm
Collana	Educazione e digitale / collana diretta da Cosimo di Bari ; 1
Altri autori (Persone)	Di Bari, Cosimoauthor
Disciplina	809.89282
Soggetti	Letteratura per ragazzi - Pedagogia
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia