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Autore	Geiser Jurgen
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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.

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