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OpenGeoSys Tutorial

Computational Hydrology III: OGS#IPhreeqc Coupled Reactive Transport Modeling

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Preface

This tutorial presents the application of the open-source software *OpenGeoSys* (*OGS*) (Kolditz et al. 2012) with a geochemical solver *PHREEQC* (Palandri and Kharaka 2004) for hydrological simulations concerning reactive transport modeling. This tutorial is a result of the close cooperation within the *OGS* community (www.opengeosys.org), and these voluntary contributions are highly acknowledged.

The book contains general information regarding the reactive transport modeling and a step-by-step setup of models with *OGS* and *PHREEQC*, and related components such as *GINA_OGS*, *ParaView*, and *Data Explorer*. Benchmark examples are presented in detail.

This book is intended primarily for graduate students and applied scientists who deal with reactive transport modeling. It is also a valuable source of information for professional geo-scientists wishing to advance their knowledge in numerical modeling of hydrological processes including reactive transport modeling.

This tutorial is the third in a series that will represent further applications of computational modeling in hydrological sciences.

- Computational Hydrology I: Groundwater flow modeling, Sachse et al. (2015), DOI 10.1007/978-3-319-13335-5, http://www.springer.com/de/book/9783319133348
- Computational Hydrology II: Groundwater quality modeling, Sachse et al. (2017), DOI 10.1007/978-3-319-52809-0, http://www.springer.com/gp/book/9783319528083
- Computational Hydrology III: OGS#IPhreeqc coupled reactive transport modeling, Jang et al. (2017, this volume)

These contributions are related to a similar publication series in the field of environmental and energy sciences:

- Geoenergy Modeling I: Geothermal Processes in Fractured Porous Media, Böttcher et al. (2016), DOI 10.1007/978-3-319-31335-1, http://www.springer.com/de/book/9783319313337

- Geoenergy Modeling II: Shallow Geothermal Systems, Shao et al. (2016), DOI 10.1007/978-3-319-45057-5, http://www.springer.com/de/book/9783319450551
- Geoenergy Modeling III: Enhanced Geothermal Systems, Watanabe et al. (2016), DOI 10.1007/978-3-319-46581-4, http://www.springer.com/de/book/9783319465791
- Geoenergy Modeling IV: Computational Geotechnics: Storage of Energy Carriers, Nagel et al. (2017), DOI 10.1007/978-3-319-56962-8, http://www.springer.com/gp/book/9783319569604
- Geoenergy Modeling V: Models of Thermochemical Heat Storage, Lehmann et al. (2017*)
- OGS Data Explorer, Rink et al. (2018*),

(*publication time is approximated).

Leipzig, Germany
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O. Kolditz, S. Bauer, L. Bilke, N. Böttcher, J.O. Delfs, T. Fischer, U.J. Görke, T. Kalbacher, G. Kosakowski, C.I. McDermott, C.H. Park, F. Radu, K. Rink, H. Shao, H.B. Shao, F. Sun, Y.Y. Sun, A.K. Singh, J. Taron, M. Walther, W. Wang, N. Watanabe, Y. Wu, M. Xie, W. Xu, B. Zehner, OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (thm/c) processes in porous media. Environ. Earth Sci. **67**, 589–599 (2012). doi:10.1007/s12665-012-1546-x. https://doi.org/10.1007/s12665-012-1546-x

J.L. Palandri, Y.K. Kharaka, A compilation of rate parameters of watermineral interaction kinetics for application to geochemical modeling. Technical report, 2004

The original version of the book was revised: Missed out corrections have been incorporated. The erratum to the book is available at http://dx.doi.org/10.1007/978-3-319-67153-6_8

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