

SPRINGER BRIEFS IN EARTH SYSTEM SCIENCES

Eunseon Jang
Johannes Boog
Wenkui He
Thomas Kalbacher

OpenGeoSys Tutorial

Computational Hydrology III: OGS#IPhreeqc Coupled Reactive Transport Modeling

EXTRAS ONLINE



Springer

SpringerBriefs in Earth System Sciences

Series editors

Gerrit Lohmann, Bremen, Germany

Lawrence A. Mysak, Montreal, Canada

Justus Notholt, Bremen, Germany

Jorge Rabassa, Ushuaia, Argentina

Vikram Unnithan, Bremen, Germany

More information about this series at <http://www.springer.com/series/10032>

Eunseon Jang · Johannes Boog
Wenkui He · Thomas Kalbacher

OpenGeoSys Tutorial

Computational Hydrology III: OGS#IPhreeqc
Coupled Reactive Transport Modeling

Eunseon Jang
Department of Environmental Informatics
Helmholtz Centre for Environmental
Research—UFZ
Leipzig, Sachsen
Germany

Johannes Boog
Department Centre for Environmental
Biotechnology
Helmholtz Centre for Environmental
Research—UFZ
Leipzig, Sachsen
Germany

Wenkui He
Dr. Knoell Consult GmbH
Mannheim, Baden-Württemberg
Germany

Thomas Kalbacher
Department of Environmental Informatics
Helmholtz Centre for Environmental
Research—UFZ
Leipzig, Sachsen
Germany

Additional material to this book can be downloaded from <http://extras.springer.com>.

ISSN 2191-589X ISSN 2191-5903 (electronic)
SpringerBriefs in Earth System Sciences
ISBN 978-3-319-67152-9 ISBN 978-3-319-67153-6 (eBook)
<https://doi.org/10.1007/978-3-319-67153-6>

Library of Congress Control Number: 2017955242

© The Author(s) 2018, corrected publication 2018

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer International Publishing AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

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](https://doi.org/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](https://doi.org/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:

- Geoenery Modeling I: Geothermal Processes in Fractured Porous Media, Böttcher et al. (2016), DOI [10.1007/978-3-319-31335-1](https://doi.org/10.1007/978-3-319-31335-1), <http://www.springer.com/de/book/9783319313337>

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

(*publication time is approximated).

Leipzig, Germany
August 2017

Eunseon Jang
Johannes Boog
Wenkui He
Thomas Kalbacher

References

- 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). <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*

Acknowledgements

We deeply acknowledge the continuous scientific and financial support to the *OpenGeoSys* development activities by the following institutions:



We would like to express our sincere thanks to the UFZ graduate school HIGRADE in providing funding the *OpenGeoSys* training course at the Helmholtz Centre for Environmental Research GmbH—UFZ.

We also wish to thank the *OpenGeoSys*-developer group (ogs-devs@googlegroups.com) and the users (ogs-users@googlegroups.com) for their technical support.

Contents

1 Introduction	1
Thomas Kalbacher	
1.1 Reactive Transport Modeling (RTM)	1
1.2 Reactive Nitrogen in the Environment	2
1.3 Coupling of Code and Software	3
References	4
2 Methods	7
Eunseon Jang and Wenkui He	
2.1 OpenGeoSys (OGS)	7
2.2 PHREEQC and IPhreeqc Module	9
2.3 OGS#IPhreeqc Coupling Scheme	9
References	12
3 Software Requirements and Installation	15
Eunseon Jang and Johannes Boog	
3.1 Preprocessing I: GINA	16
3.2 Preprocessing II: GMSH and OGS Data Explorer	17
3.3 Processing: OGS#IPhreeqc	18
3.3.1 Download the Source Code	18
3.3.2 Configure the Building Project	19
3.3.3 Compile the Code	20
3.4 Post-processing: ParaView	21
References	23
4 File Description	25
Eunseon Jang and Thomas Kalbacher	
4.1 OGS Input Files	25
4.2 PHREEQC Input Files	27
Reference	29

- 5 Code Verification: Engesgaard Benchmark** 31
 - Wenkui He
 - 5.1 Benchmark Description 31
 - 5.2 Model Setup 32
 - 5.3 Simulation Results 34
 - References 34

- 6 Application: Nitrate Reduction Processes** 37
 - Eunseon Jang
 - 6.1 Introduction 37
 - 6.2 Background 37
 - 6.3 Model Components and Governing Equations 38
 - 6.3.1 Model Scenario 38
 - 6.3.2 Groundwater Flow and Solute Transport Equations 39
 - 6.3.3 Geochemical System 40
 - 6.4 Model Setup 42
 - 6.4.1 Preprocessing 42
 - 6.4.2 Model Execution 57
 - 6.4.3 Post-processing 59
 - 6.5 Simulation Results 59
 - References 60

- 7 Application: Treatment Wetlands** 63
 - Johannes Boog
 - 7.1 Introduction 63
 - 7.2 Background 63
 - 7.3 Model Components and Governing Equations 65
 - 7.3.1 Experimental System 65
 - 7.3.2 Water Flow and Mass Transport 65
 - 7.3.3 Biodegradation 66
 - 7.4 Practical Model Setup 69
 - 7.4.1 Preprocessing 69
 - 7.4.2 Model Execution 83
 - 7.4.3 Post-processing 87
 - 7.5 Simulation Results 87
 - References 89

- Erratum to: OpenGeoSys Tutorial** E1

- Appendix A: OpenGeoSys v5 Keywords Description** 91