Terrestrial Environmental Sciences

Olaf Kolditz
Thomas Nagel
Hua Shao
Wenqing Wang
Sebastian Bauer *Editors*

Thermo-Hydro-Mechanical-Chemical Processes in Fractured Porous Media: Modelling and Benchmarking

From Benchmarking to Tutoring

Springer

Terrestrial Environmental Sciences

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ISSN 2363-6181 ISSN 2363-619X (electronic)
Terrestrial Environmental Sciences
ISBN 978-3-319-68224-2 ISBN 978-3-319-68225-9 (eBook)
https://doi.org/10.1007/978-3-319-68225-9

Library of Congress Control Number: 2018930139

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 is the fourth volume of the THMC benchmark book series dealing with benchmarks and examples of thermo-hydro-mechanical-chemical processes in fractured porous media:

1. http://www.springer.com/de/book/9783642271762
2. http://www.springer.com/de/book/9783319118932
3. http://www.springer.com/de/book/9783319292236
4. http://www.springer.com/de/book/9783319682242 (this volume)

Recently, the benchmark books became items of the new book series in “Terrestrial Environmental Sciences” http://www.springer.com/series/13468.

The present book is subtitled “From Benchmarking to Tutoring.” The material from benchmark books has also been prepared for tutorials which build the foundation for teaching purposes and training courses as well, highlighting the multipurpose benefits from continuous benchmarking.

The book structure again follows the “classic” scheme, presenting first single processes and then coupled processes with increasing complexity. The list of symbols and an index you will find at the end of the book. With this book, we also want to award the work of merit of distinguished scientists in the field “Modelling and Benchmarking of THMC Processes.”

Along with this version, we also provide the input files for self-exercising and enhanced reproducibility. These can be found at the OGS community page http://docs.opengeosys.org/books (Fig. 1). Software engineering has been further improved by integrated Ctests and direct GitHub-Links for OGS code references (Sect. A.2).

The OGS Tutorial series has been extended by additional volumes on Computational Hydrology (I–III) and Geoenergy Modelling (I–III). A new section on Computational Geotechnics was opened starting with a volume on the Storage of Energy Carriers followed by a volume on Models of Thermochemical Heat Storage:

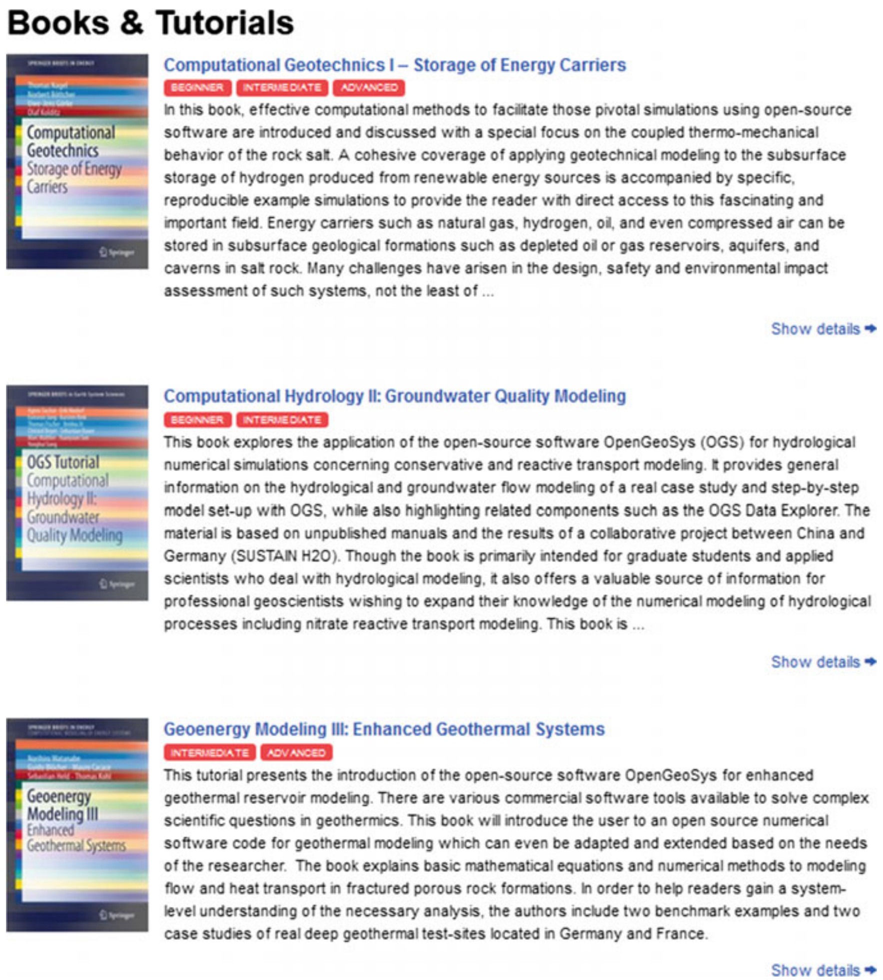
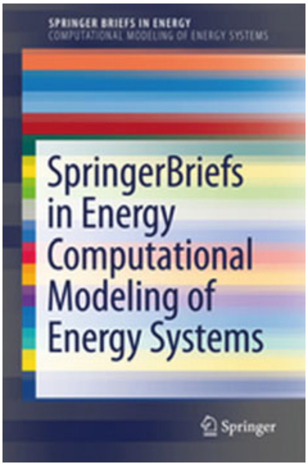


Fig. 1 Benchmark books and related tutorials

- "Computational Hydrology I: Groundwater Flow Modeling" (Sachse et al. 2015)
  http://www.springer.com/de/book/9783319133348,
- "Computational Hydrology II: Groundwater Quality Modeling" (Sachse et al. 2017)
  http://www.springer.com/us/book/9783319528083,
- "Computational Hydrology III: OGS#IPhreeqc Coupled Reactive Transport Modeling" (Jang et al. 2018)
  http://www.springer.com/us/book/9783319671529,
- "Geoenergy Modeling I: Geothermal Processes in Fractured Porous Media" (Boettcher et al. 2016)
  http://www.springer.com/de/book/9783319313337,

- "Geoenergy Modeling II: Shallow Geothermal Systems" (Shao et al. 2017) http://www.springer.com/us/book/9783319450551,
- "Geoenergy Modeling III: Enhanced Geothermal Systems" (Watanabe et al. 2017) http://www.springer.com/us/book/9783319465791,
- "Computational Geotechnics—Storage of Energy Carriers" (Nagel et al. 2017a) http://www.springer.com/de/book/9783319313337,
- "Models of Thermochemical Heat Storage" (Lehmann et al. 2018) http://www.springer.com/de/book/9783319715216,



For geo- and energy-related tutorials, a new subseries on "Computational Modeling of Energy Systems" has been launched edited by Thomas Nagel and Haibing Shao. "This subseries puts a spotlight on advanced computational and theoretical methods, tools, and frameworks for the design, analysis, optimization, and assessment of a diverse range of energy technologies and systems. The intention is to make the methods transparent and to allow engineers and scientists from different disciplines to enter the field of energy research enabling them to perform meaningful simulations for the advancement of clean and secure energy systems."

(http://www.springer.com/series/15395)

Enjoy reading, exercising and benchmarking.

Leipzig and Dresden, Germany	Olaf Kolditz
Leipzig and Dublin, Germany	Thomas Nagel
Leipzig, Germany	Wenqing Wang
Hanover, Germany	Hua Shao
Kiel, Germany	Sebastian Bauer
November 2017	

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Dr. Uwe-Jens Görke[1]

We would like to honor Dr. Uwe-Jens Görke for his scientific contribution to the field of computational mechanics and in particular for his tremendous engagement supporting young scientists and community efforts.

Uwe studied Mathematics and Continuum Mechanics (Theoretical Mechanics) at the Kharkov State University in the former Soviet Union (now Ukraine). At that time our paths crossed for the first time. Dr. Uwe-Jens Görke received his Ph.D. in 1987 from the College of Engineering (Zwickau) in the field of computational mechanics focusing on viscoelastic material models at large strains. Uwe then worked as a Postdoc at the Institute of Mechanics of the Academy of Sciences of the GDR (Karl-Marx-Stadt), where our ways crossed again, when Olaf Kolditz did his my Ph.D. (Uwe was always ahead of Olaf Kolditz …). He worked at several research institutes (Fraunhofer Institute for Structural Durability in Darmstadt) and universities (Chemnitz University of Technology) with main research topics in material modelling, parameter identification, and computational mechanics for solid and porous media with applications in industry and bioengineering. Uwe was also a visiting scientist at the AO Research Institute in Davos (Switzerland) which is dealing with applied Preclinical Research and Development within trauma and disorders of the musculoskeletal system and translation of this knowledge to achieve more effective patient care worldwide. Uwe was working there in the field of biomechanics.

Since 2008, Uwe has been a researcher at the Helmholtz Centre for Environmental Research - UFZ. His research portfolio includes continuum mechanics applied to coupled processes in porous media, thermodynamically consistent material models for inelastic solid structures at large strains, finite element method for thermo-hydro-mechanical coupled processes in porous media,

[1] Photo by Andre Künzelmann, UFZ.

porous media applications in geo- and biomechanics. His current research focuses on coupled processes in the subsurface, with a particular interest in geomechanics and material modelling. Since 2012, Uwe is senior scientist and deputy head of the Department of Environmental Informatics and now mainly involved in project management issues.

Uwe belongs to the editor team of the book series "Thermo-Hydro-mechanical-Chemical Processes in Fractured-Porous Media: Modelling and Benchmarking." From this volume, Uwe passes his editorship to Thomas Nagel. We are very grateful to Uwe for his editorial work. And with this opportunity, we would like to thank Uwe deeply for his contribution to porous media science and his support and engagement for the community and promotion of young scientists.

We very much appreciate the contributions to Uwe's Laudatio by two of his academic teachers and longtime companions.

Prof. Dr. sc. techn. Dr. E. h. H. Günther (Chemnitz, Former Director of the Institute of Mechanics with the Academy of Sciences of the GDR)

"Nach dem Studium in der Fachrichtung Mathematik und Mechanik der Universität Charkow und dem Diplom-Abschluss auf dem Gebiet der Kontinuumsmechanik begann Uwe Görke seine Tätigkeit am Lehrstuhl für Technische Mechanik der Ingenieurhochschule Zwickau (heute Westsächsische Hochschule Zwickau). Im Mittelpunkt standen Untersuchungen zu großen Deformationen in der Festkörpermechanik und 1982 promovierte er mit einer Arbeit zur Viskoelastizität kompressibler Werkstoffe. Die Ergebnisse wurden in ein hauseigenes FEMProgramm implementiert und erfolgreich auf Praxisprobleme wie die Berechnung von Hochdrucklippendichtungen und des Spannungs- und Dehnungsverhalten von Patellaknorpel angewendet. Hinzukamen numerische und experimentelle Untersuchungen zur Materialparameteridentifikation aus Relaxationsversuchen. Biomechanische Probleme weicher Gewebe standen immer wieder in seinem Interessenfeld, auch nach seinem Wechsel an das Institut für Mechanik der damaligen Akademie der Wissenschaften. So entstand letztlich unter seiner wesentlichen Mitwirkung, ein nichtlineares, modulares Materialmodell für das komplexe mechanische Verhalten biologischer Gewebe bei großen Deformationen, einschließlich Viskosität, Kompressibilität, Porosität, Isotropie und Anisotropie sowie von biologischen Vorgängen wie Osmose und Gewebe-Remodellierung. Dieses Modell wurde erfolgreich auf biomedizinische Problemstellungen des AO Research Institute Davos und des Rush University Medical-Center Chicago angewendet. Sein außerordentliches kreatives und kooperatives Managment, auch bei der FEM Implementierung, hat wesentlich zum Erfolg der Projekte beigetragen."

Prof. Dr.-Ing. habil. Reiner Kreißig (Chemnitz, Former Chair of Solid Mechanics at TU Chemnitz)

Scientific contributions from Dr.-Ing. Uwe-Jens Görke during his work at the professorship of Solid Mechanics at Chemnitz University of Technology in the years 1995–2007.

Dr. Görke has worked at the professorship Solid Mechanics mainly in research. Particularly noteworthy are his excellent research results, the partial supervision of Ph.D. students, and his contribution to several research proposals to the German Science Foundation DFG (e.g., Collaborative Research Centre (SFB) 393, Package Proposals 47 and 273).

As a scientist in SFB 393, Dr. Görke was substantially involved in the development of the in-house finite element code SPC-PM2AdNl for solving of nonlinear problems of continuum mechanics. His priorities touched many advanced topics in the field of computational mechanics, especially

- the theoretical development and numerical realization of appropriate material laws for elastoplasticity,
- the numerical solution of the nonlinear initial-boundary value problem,
- the hierarchical adaptive strategy (error estimation with respect to the equilibrium, error indicator with respect to the yield condition, mesh refinement and/or coarsening, transfer of the field variables to newly generated nodes and integration points),
- identification of the material parameters based on the analysis of inhomogeneous displacement fields (application of a nonlinear deterministic optimization approach (Levenberg-Marquardt method) for a least squares type objective function, semianalytical sensitivity analysis for the determination of the gradient of the objective function).

The development of a generalized substructure approach based on the ideas of Mandel and Dafalias was supported by Dr. Görke. In this approach, a so-called substructure configuration, which is established in addition to the usual configurations, representing the kinematics of the continuum, is defined. The substantial advantage of this modelling concept lies in its thermodynamic consistency. Aside from the theoretical work itself, the numerical realization of related problems was realized.

In the DFG priority program SPP 1146, Dr. Görke was involved in the simulation of incremental forming processes based on the material model with a substructure approach. The theoretical foundation for the modelling of coupled thermomechanical processes was developed and numerically realized in the in-house finite element code PM2AdNl. The material model is characterized by a comparatively low number of material parameters. These were determined within a gradient-based, nonlinear optimization method as described above.

Coupled multiphysics problems (hyperelastic, nearly incompressible materials, and biphasic saturated porous media at large strains) formed an additional main focus of the work of Dr. Görke. Special linearization techniques have been used to solve these problems. After spatial discretization, a global system for the incremental form of the initial-boundary problem within the framework of a stable mixed U/p-c finite element approach was defined. The global system is solved using an iterative solver with hierarchical preconditioning. Adaptive mesh evolution is controlled by a residual a posteriori error estimator.

The above results have been published in five Preprints of the SFB 393 and five Scientific Computing Preprints (www.tu-chemnitz.de/mathematik/).

Symbols

Greek Symbols

α	Biot constant (–)
α	Thermal expansion coefficient (K^{-1})
α	Intergranular radius (–)
α	Van Genuchten parameter (m^{-1})
α_k	Kinetic isotope fractionation factor (–)
α_L	Longitudinal dispersion length (m)
α_T	Transversal dispersion length (m)
β	Cubic thermal expansion coefficient (K^{-1})
β_c	Burial constant (–)
χ	Bishop coefficient (–)
2δ	Fault width (m)
Δ	Half of aspect ratio (–)
γ	Activity coefficient for dissolved species (–)
γ	Dimensionless temperature (–)
Γ	Domain boundary (–)
$\boldsymbol{\epsilon}$	Strain tensor (–)
$\dot{\epsilon}$	Strain rate (s^{-1})
ϵ	Length scale (m)
ϵ	Isotope enrichment factor (–)
ϵ	Strain (–)
ϵ_v	Volume plastic strain (–)
η	Porosity (–)
η_M	Maxwell viscosity (Pa d)
η_K	Kelvin viscosity (Pa d)
γ	Activity coefficient for dissolved species (–)
γ_l	First-order degradation rate (day^{-1})
κ	Thermal conductivity (W m^{-1} K^{-1})
λ_c	Virgin compression index (–)
λ	Lamé coefficients (GPa)

λ_p	Hardening parameter (–)
λ	Thermal conductivity (W m^{-1} K^{-1})
λ_{arith}	Arithmetic effective thermal conductivity (W m^{-1} K^{-1})
λ_b	Bulk thermal conductivity (W m^{-1} K^{-1})
λ_{eff}	Effective thermal conductivity (W m^{-1} K^{-1})
λ_f	Fluid thermal conductivity (W m^{-1} K^{-1})
λ_{geom}	Geometric effective thermal conductivity (W m^{-1} K^{-1})
λ_{harm}	Harmonic effective thermal conductivity (W m^{-1} K^{-1})
λ_{pm}	Thermal conductivity of porous medium (W m^{-1} K^{-1})
λ_s	Solid thermal conductivity (W m^{-1} K^{-1})
μ	Lamé coefficients (GPa)
μ	Dynamic viscosity (Pa s)
μ_0	Base dynamic viscosity (Pa s)
ν	Poisson number (–)
Q_ω	Source/sink term (kg m^{-3} s^{-1})
ω	Intergranular thickness (m)
ω	Saturation index (–)
ϕ	Porosity (–)
ϕ	Friction angle (deg)
ψ	Dilatancy angle (deg)
ρ	Density (kg m^{-3})
ϱ_{SR}	Real density of solid (kg m^{-3})
ϱ_{LR}	Real density of liquid (kg m^{-3})
ϱ_{IR}	Real density of ice (kg m^{-3})
ρ_s	Density of solid (kg m^{-3})
ρ_w	Density of water (kg m^{-3})
ρ_d^s	Density of bentonite bulk (kg m^{-3})
ρ_0	Base fluid density (kg m^{-3})
σ	Cauchy stress tensor (Pa)
σ_{V}	Von Mises equivalent stress (Pa)
σ_{con}	Confining stress (Pa)
σ_{eff}	Effective stress (Pa)
σ	Effective stress (Pa)
σ_{max}^{sw}	Tested maximum swelling stress (Pa)
σ_a	Contact stress (Pa)
σ_c	Critical stress (Pa)
ν_{M}	Maxwell viscosity tensor (Pa d)
ν_{K}	Kelvin viscosity tensor (Pa d)

Roman Symbols

a	Specific surface area (m^2 m^{-3})
a^σ	Activity of stressed solid (–)
$\dot{a}$	Effective diameter of ion (m)
A	Surface area (m^2)
$\mathbf{b}$	Body force vector (N)
b_h	Fracture hydraulic aperture (m)
b_m	Fracture mechanical aperture (m)
c	Normalized concentration (–)
c	Concentration (kg m^{-3})
c	Cohesion (–)
C^h_{eq}	Solubility under hydrostatic pressure (mol m^{-3})
C_i	Intergranular concentration (mol m^{-3})
C_p	Pore-space concentration (mol m^{-3})
Cr	Courant number (–)
c_f	Specific fluid heat capacity (J kg^{-1} k^{-1})
c_p	Heat capacity (J kg^{-1} k^{-1})
Cp	Heat capacity (J kg^{-1} k^{-1})
d	Order parameter (–)
D	Diffusivity coefficient (m^2 s^{-1})
D_f	Intergranular diffusion coefficient (m^2 s^{-1})
E	Young's modulus (Pa)
e	Void ratio (–)
g	Gravitational coefficient (m s^{-2})
g	Plastic potential (J)
$\mathbf{g}$	Gravity vector (m s^{-2})
$\mathbf{g}$	Gravitational acceleration (m s^{-2})
g_c	Fracture toughness (N m^{-1})
G	Gibbs energy (J)
G	Gibbs energy (J mol^{-1})
G	Shear modulus (Pa)
G_F	Plastic potential (J)
G_M	Maxwell shear modulus (–)
G_K	Kelvin shear modulus (–)
H	Fault height (m)
H_{pw}	Pipe water level (m)
h	Hardening parameter (–)
h_c	Thickness of colmation layer (m)
h_f	Freshwater hydraulic head (m)
h_s	Saltwater hydraulic head (m)
$\triangle h_I$	Specific enthalpy of fusion (J)
I	Ionic strength (–)
I_1	First principal invariant of the stress tensor (Pa)
I_r	Friction slope (–)

I_s	Bottom slope (–)
J_2	Second principal invariant of the deviatoric stress tensor (Pa^2)
J_3	Third principal invariant of the deviatoric stress tensor (Pa^3)
k	Residual stiffness parameter (–)
$\mathbf{k}$	Permeability tensor (m^2)
$\mathbf{k}$	Permeability tensor ($m\ s^{-1}$)
$\mathbf{K}$	Intrinsic permeability (m^2)
k_c	Swelling/recompression index (–)
K_{eq}	Equilibrium constant (–)
K_{M}	Maxwell bulk modulus (–)
K_{n}	Normal stiffness ($Pa\ m^{-1}$)
K_{s}	Shear stiffness ($Pa\ m^{-1}$)
$K_{\mathrm{r}}el$	Relative permeability (m^2)
k_{s}	Saturated hydraulic conductivity ($m\ d^{-1}$)
k^+	Dissolution rate constant ($mol\ m^{-2}\ s^{-1}$)
k°	Reaction rate constant ($mol\ m^{-2}\ s^{-1}$)
M	Kinetic coefficient ($mm^2\ N^{-1}\ s^{-1}$)
M	Slope of critical state line (–)
M_w	Molecular mass of water vapor (18.016 $g\ mol^{-1}$)
n	Porosity ($m^3\ m^{-3}$)
n	Van Genuchten parameter (–)
m	Van Genuchten parameter (–)
p	Pressure ($kg\ s^{-1}\ m^{-1}$)
p	Pressure (Pa)
P	Load (Pa)
P_c	Capillary pressure (Pa)
p_{s}	Mean stress (Pa)
p_{scn}	Isotropic pre-consolidation pressure (Pa)
Pe	Péclet number (–)
q	Source/sink term (–)
q	Shear stress (Pa)
q	Heat source (W)
q	Darcy velocity ($m\ s^{-1}$)
$\mathbf{q}$	Darcy velocity vector ($m\ s^{-1}$)
Q	Ion activity product (–)
Q_{leak}	Leakage flow ($m^3\ s^{-1}$)
q_{T}	Heat flux through unit area ($W\ m^{-2}$)
R	Universal gas constant (8.31432 $J\ mol^{-1}\ K^{-1}$)
R_c	Contact area ratio (–)
Ra	Rayleigh number (–)
$\mathrm{Ra}_{\mathrm{crit}}$	Critical Rayleigh number (–)
s	Soil suction (kPa)
S	Saturation (–)
S	Storage ($1\ Pa^{-1}$)
S_{e}	Effective saturation (–)

S_{max}	Maximum water saturation (–)
S_r	Residual saturation (–)
$\mathrm{S_r}$	Residual water saturation (–)
SA	Reactive surface area (m^2)
t	Time (s)
T	Temperature (K)
T	Absolute temperature (K)
T_c	Top temperature (cold) (K)
T_h	Bottom temperature (hot) (K)
T_{init}	Initial temperature (K)
T_v	Approximation temperature (K)
u	Displacement (m)
$\mathbf{u}$	Displacement vector (m)
v	Velocity (m s^{-1})
V	Volume (m^3)
V_m	Molar volume (m^3 mol^{-1})
V_u	Cell volume (m^3)
w	Margules parameter (J mol^{-1})
X	Molar fraction (–)
Z	Ionic integer charge (–)
Z	Charge (–)

Indices

$\parallel$	Co-linear direction
$\perp$	Orthogonal direction
e	Efficient value
f	Fluid
f	Fracture
w	Water
s	Solid
0	Reference value

Operators

div, $\nabla\cdot$	Divergence operator
grad, ∇	Nabla, gradient operator
tr	Trace

Part I
Introduction

Chapter 1
Introduction

Olaf Kolditz, Thomas Nagel and Hua Shao

1.1 Recent Developments in THMC Research

Olaf Kolditz, Thomas Nagel, Hua Shao

In this section we discuss recent literature in thermo-hydro-mechanical-chemical (THMC) analysis particularly in fractured-porous media. Figure 1.1 depicts the quantitative development of Scopus listed publications in the field and highlights the increasing interest in THMC research.

THMC research is mainly related to geoscientific and environmental applications based on porous media approaches. A few works are dedicated to material research.

1.2 Events

In 2017 several important events took place related to THMC research such as the Mont Terri Technical Meeting 2017 in Porrentruy (Switzerland) and the DECOVALEX 25th Anniversary in Stockholm (Sweden) (see Sect. 1.2).

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O. Kolditz et al. (eds.), *Thermo-Hydro-Mechanical-Chemical Processes in Fractured Porous Media: Modelling and Benchmarking*,
Terrestrial Environmental Sciences, https://doi.org/10.1007/978-3-319-68225-9_1

Porrentruy: The Mont Terri Technical Meeting (TM-35) from 08–09.02.2017 was held for annual review of selected ongoing experiments but also for discussion of new experiments which will be designed within the framework of rock lab extension later on this year. This meeting was also dedicated to celebrate the 20th anniversary of the Mont Terri Underground Research Laboratory (URL) being an excellent place of international applied research in clay rocks world-wide for over 2 decades. Due to this occasion, a Special Issue was published in the *Swiss Journal of Geosciences* "Mont Terri rock laboratory, 20 years of research: introduction, site characteristics and overview of experiments" Bossart et al. (2017) compiling recent research works from the project participants.

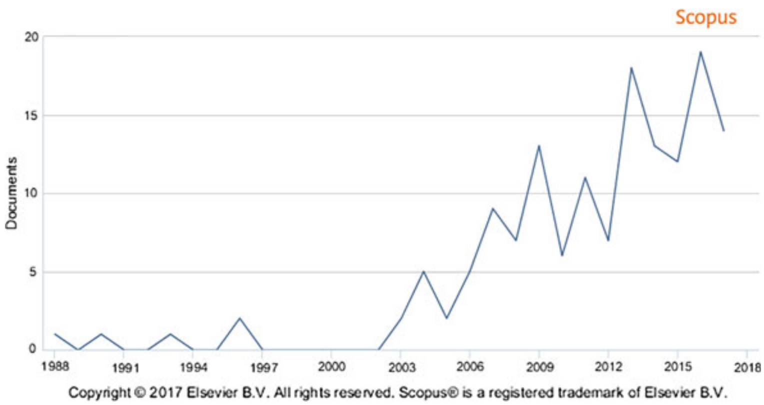

Fig. 1.1 Increase of THMC papers over years (source: Scopus)

Stockholm: The 3rd DECOVALEX-2019 workshop from 25–28.04.2017 in Sweden's capital was more than the ordinary status meeting with progress reports about the seven individual tasks of the project phase 7 ...

... it was also dedicated to the celebration of the DECOVALEX's 25th anniversary. To this purpose the pioneers of DECOVALEX - DEvelopment of COupled models and their VALidation against EXperiments - were invited for a panel discussion to explain the unusual success story of this project (Ove Stephansson, Ivars Neretnieks, Johan Andersson, Ki-Bok Min, Chin-Fu Tsang, from left to right).

1.3 Literature Review

A literature review in Scopus (2016–early 2018) yielded the following topics in THMC analyses:

- General and review works (Sect. 1.3.1),
- Nuclear and chemo-toxic waste management, landfills Sect. 1.3.2,
- Geological CO2 storage (Sect. 1.3.3),
- Geothermal energy systems (Sect. 1.3.4),
- Reservoir exploitation and drilling (Sect. 1.3.5).

Nuclear waste management is the most frequent and intensive discussed topic in recent literature.

1.3.1 General and Review Works

Wang et al. (2017) provide a comprehensive literature review on the simulation techniques for describing flow processes in shale and tight gas reservoirs. "The capabilities of existing reservoir simulation tools are discussed in terms of numerical methods (finite difference, finite element, explicit/implicit scheme, sequentially and fully coupled schemes), fluid flow behavior (Darcy and non-Darcy flow, desorption, Klinkenberg effect and gas slip flow, transitional flow, Knudsen diffusion), reservoir rock properties (pore size distribution, fractures, geomechanics), coupling schemes, modeling scale, and computational efficiency." The authors also elaborate on pros and cons of pore-scale modeling, e.g. using lattice-Boltzmann approaches.

Wang (2017) present a fully coupled THMC model for fracture opening and closure by explicitly accounting for stress concentration on aperture surface, stress-activated mineral dissolution, pressure solution at contacting asperities, and channel flow dynamics. They showed that "a tangential surface stress created by a far-field compressive normal stress may play an important role in controlling fracture aperture evolution in a stressed geologic medium."

THMC simulation is also important for the understanding of fundamental Earth system processes such as lithospheric deformation, e.g. for analysis of Episodic Tremor and Slip (ETS) events. Veveakis et al. (2017) consider THMC instabilities triggered by the fluid release reactions in fault zones. "Data from ETS sequences in subduction zones reveal a geophysically tractable temporal evolution with no access to the fault zone." Alevizos et al. (2017) present a fundamental theoretical analysis on the important lithosphere deformation mechanism of creep enhanced by fluid-release reactions. "This mechanism features surprisingly rich dynamics stemming from the feedback between deformation induced fluid release through mineral breakdown reactions (dissolution) and fluid cementation into a solid matrix (precipitation) when the tectonic forces are locally relaxed." They show that TM feedback processes in the temperature and pressure evolution and the resulting feedback between fluid flow and mechanical deformation (HM processes) result in a highly dynamic system.

Faoro et al. (2016) present a fundamental study concerning permeability changes in fractured rocks due to THMC processes. "These experiments examine the influence of thermally and mechanically activated dissolution of minerals on the mechanical (stress/strain) and transport (permeability) responses of fractures." The data base relies on heated (25 °C up to 150 °C) flow-through experiments on fractured core samples of Westerly granite. The measured efflux of dissolved mineral mass provides a record of the net mass removal, which is correlated with observed changes in relative hydraulic fracture aperture. The authors argue "that at low temperature and high stresses, mechanical crushing of the asperities and the production of gouge explain the permeability decrease although most of the permeability is recoverable as the stress is released. While at high temperature, the permeability changes are governed by mechanical deformation as well as chemical processes, in particular, we infer dissolution of minerals adjacent to the fracture and precipitation of kaolinite."

Fig. 1.2 DECOVALEX tasks explore different complexity of T-H-M/C exercises based on experimental evidence. Fully coupled problems have been investigated e.g. by Bond et al. (2017, 2016), Pfeiffer et al. (2016), Pan et al. (2016), McDermott et al. (2015)

Rutqvist (2016) provides an overview of TOUGH-based geomechanics models and summarizes the history of TOUGH-FLAC3D developments in the past 15 years for various geoengineering applications such as “geologic CO2 sequestration, enhanced geothermal systems, unconventional hydrocarbon production, and most recently, related to reservoir stimulation and injection-induced seismicity.”

1.3.2 Nuclear Waste Management

The scientific results of the previous **DECOVALEX**-2015 phase have been published recently as a Thematic Issue in *Environmental Earth Sciences*.[1] The volume contains 18 research papers describing details of Tasks A, B, C1, C2 as well as summarizing the model comparison exercises (Fig. 1.2).

A short introduction to the ongoing **DECOVALEX**-2019 can be found in Sect. 1.5 and through the related website.[2]

“Geologic repositories for radioactive waste are designed as multi-barrier disposal systems that perform a number of functions including the long-term isolation and containment of waste from the human environment, and the attenuation of radionuclides released to the subsurface. The rock laboratory at **Mont Terri** (canton Jura,

[1] https://link.springer.com/journal/12665/topicalCollection/AC_4afd5d3151e292e32fb5583c8a0d4b9a/page/1.

[2] www.decovalex.org.

Switzerland) in the Opalinus Clay plays an important role in the development of such repositories." Bossart et al. (2017) summarized the experimental results gained in the last 20 years to study the possible evolution of a repository and investigate processes closely related to the safety functions of a repository hosted in a clay rock. "At the same time, these experiments have increased the general knowledge of the complex behaviour of argillaceous formations in response to coupled hydrological, mechanical, thermal, chemical, and biological processes". Numerous research aspects are covered in a Special Issue of the *Swiss Journal of Geosciences*: bentonite buffer emplacement, high-pH concrete-clay interaction experiments, anaerobic steel corrosion with hydrogen formation, depletion of hydrogen by microbial activity, and finally, release of radionuclides into the bentonite buffer and the Opalinus Clay barrier. "The research at Mont Terri carried out in the last 20 years provides valuable information on repository evolution and strong arguments for a sound safety case for a repository in argillaceous formations."

Bernier et al. (2017) pointed out the key THMC processes that might influence radionuclide transport in a disposal system and its surrounding environment, considering the dynamic nature of these processes. These THMC processes have a potential impact on safety; it is important "to identify and to understand them properly when developing a disposal concept to ensure compliance with relevant safety requirements."

Lu et al. (2017a) and Lu and Fall (2017) developed a coupled thermo-hydro-mechanical-chemical (THMC)-visco-plastic cap model to characterize the behavior of cementing mine backfill material under blast loading. "The model is coupled to a Perzyna type of visco-plastic model with a modified smooth surface cap envelope and a variable bulk modulus, in order to reasonably capture the nonlinear and rate-dependent behaviors of the cemented tailings backfill under blast loading." The proposed model allows for a better understanding of hydrating cemented backfill under blasting conditions, and also practical risk management of backfill structures associated with dynamic environments. Ghirian and Fall (2016) conducted experimental work using a pressure cell apparatus to study the long-term hydro-mechanical behaviour of cemented paste backfill (CPB).

Bente et al. (2017) deal with a model for time-dependent compaction of porous materials with applications to degradation-induced settlements in municipal solid waste landfills. The Theory of Porous Media is used as continuum mechanical framework; for kinematic description, large strain continuum mechanics is applied.

Nishimura (2016) investigated compacted bentonite as an important component of engineered barrier systems. They present a new method of determining creep behavior and failure of compacted bentonite under constant (or maintained) high relative humidity. THMC modeling is suggested as an appropriate analysis tool.

Abed et al. (2016) started modelling coupled THMC behaviour of unsaturated bentonite relying on the Barcelona Basic Model (BBM). "As an alternative, BBM is used alongside the Krähn's model which assumes that bentonite re-saturation is mainly driven by water vapour diffusion." Both methods have been compared with laboratory experiments based on X-ray tomography and show similar results.

Yasuhara et al. (2016b) developed a THMC numerical model to examine the long-term change in permeability of the porous sedimentary rocks (quartz-rich), in particular, the chemo-mechanical process of the pressure solution is incorporated. “The model predictions clearly showed a significant influence of the pressure dissolution on the change in permeability with time” and, therefore, are important consideration for long-term high-level radioactive waste deposition (Yasuhara et al. 2016a).

GMZ-Na-bentonite is a selected buffer material for the preliminary concept of HLW repository in China. Liu et al. (2016) investigate THMC processes for the China-Mock-up facility. “Stress evolution of the compacted bentonite may be influenced by several mechanisms, including gravity, thermal expansion induced by high temperature, and the swelling pressure generated by bentonite saturation.” The experimental results and achievements obtained from the THMC experiments provide important insight into GMZ-bentonite under realistic HLW repository conditions and the design.

1.3.3 Geological CO2 Storage

Li et al. (2016a): “Carbon dioxide (CO_2) capture and storage (CCS) is considered widely as one of promising options for CO2 emissions reduction, especially for those countries with coal-dominant energy mix like China. Injecting and storing a huge volume of CO2 in deep formations are likely to cause a series of geomechanical issues, including ground surface uplift, damage of caprock integrity, and fault reactivation.” They present results from the Shenhua CCS demonstration project in Ordos Basin, China, which is the largest full-chain saline aquifer storage project of CO2 in Asia - a combination of CCS and overlying coal seam mining. Interferometric synthetic aperture radar (InSAR) technology was used for subsidence monitoring. THMC modeling was mainly used for geomechanical stability analysis. Li et al. (2016b) provide a comprehensive review of numerical approaches for analyzing the geomechanical effects induced by CO2 geological storage. They introduce theoretical aspects and classify numerical simulation methods for THMC analyses.

Zhang et al. (2016a, b) propose a sequentially coupled computational THMC framework for a variety of geo-applications such as CO2 geo-sequestration (CCS) and Engineered Geothermal Systems (EGS). Zhang and Wu (2016) present a practical reactive transport example with complex chemical compositions (Fig. 1.3).

1.3.4 Geothermal Energy Systems

Blöcher et al. (2016) investigate the THMC behaviour of a research well doublet consisting of the injection well E GrSk 3/90 and the production well Gt GrSk 4/05 A(2) in the deep geothermal reservoir of Groβ Schönebeck (north of Berlin, Germany)