Chapter 6
Synthesis and Outlook

Olaf Kolditz, Tuanny Cajuhi, Ralf-Michael Günther, Holger Steeb, Frank Wuttke, Keita Yoshioka, Norbert Grunwald, and Thomas Nagel

The principal interest of the GeomInt project consists of the investigation of effects on barrier integrity of three host rock formations: clay, salt and crystalline. The project focuses on distinct physical processes that can influence barrier integrity in these rocks, particularly those related to swelling and shrinkage, pressure-driven

O. Kolditz (✉)
UFZ, Helmholtz Centre for Environmental Research, Leipzig and Technische Universität Dresden, Dresden, Germany
e-mail: olaf.kolditz@ufz.de

T. Cajuhi
BGR, Federal Institute for Geosciences and Natural Resources, Hanover, Germany
e-mail: Tuanny.Cajuhi@bgr.de

R.-M. Günther
IfG Institut für Gebirgsmechanik GmbH, Leipzig, Germany
e-mail: ralf.guenther@ifg-leipzig.de

H. Steeb
UoS, University of Stuttgart, Stuttgart, Germany

F. Wuttke
CAU, Christian-Albrechts-Universität zu Kiel, Kiel, Germany
e-mail: frank.wuttke@ifg.uni-kiel.de

K. Yoshioka
UFZ, Helmholtz Centre for Environmental Research, Leipzig, Germany
e-mail: keita.yoshioka@ufz.de

UoL, University of Leoben, Leoben, Austria

N. Grunwald
UFZ, Helmholtz Centre for Environmental Research, Leipzig, Germany
e-mail: norbert.grunwald@ufz.de

T. Nagel
TUBAF, Technische Universität Bergakademie Freiberg, Freiberg, Germany
e-mail: thomas.nagel@ifgt.tu-freiberg.de

O. Kolditz et al. (eds.), *GeomInt—Discontinuities in Geosystems From Lab to Field Scale*, SpringerBriefs in Earth System Sciences,
https://doi.org/10.1007/978-3-031-26493-1_6

percolation and stress redistribution. In the first part of the project, methodologies were developed in both experimental and numerical areas (Kolditz et al. 2021b). Combined model-experiment studies (MEX) were used as the first synthesis tool. The problem classes (processes and rock types) were systematized and model and code comparisons were made for test examples (benchmarks) and laboratory experiments. A further result of the first project phase was also to systematically evaluate (advantages and disadvantages) the suitability of certain experiments and numerical methods for the individual or combined process classes (see above), which can influence the barrier effect, and to make further studies available (Kolditz et al. 2021a). In the second phase of the project, the methodical tools were used in particular for the analysis of laboratory and field experiments. Model chains (Sect. 6.1) and formation-specific workflows (Sect. 6.3) were developed as further synthesis tools, which are briefly presented below. Moreover, the GeomInt project has benefited from the outreach to various national and international activities such as the Mont Terri project, BenVaSim, DECOVALEX, and EURAD (Sect. 6.2).

6.1 Mechanical Integrity of Clay Rocks

6.1.1 Model Chains

Barrier integrity can be affected by a number of processes. In the case of gas permeation, relevant processes are highlighted in Fig. 6.1. Gases can arise e.g. from corrosion, degradation of organic compounds, setting of cement or pyrolysis. Gases initially spread out in dissolved form diffusely and advectively. At higher pressures, a gaseous phase can form, which propagates further as a multiphase flow. If the gas pressure continues to rise, mechanical damage to the rock with dilatancy and eventually propagating fractures can occur. The EURAD project is currently investigating whether this damage in clay rocks is reversible when the fluid pressures decrease and the plastic rock material converges and the fractures close again (the so-called self-sealing effect). This process chain shown in Fig. 6.1 can be mapped using new calculation methods (Grunwald et al. 2022). Dis- and continuum mechanical approaches, which were developed in GeomInt, are combined. The variational phase field (VPF) method is used for simulating fracture propagation processes (Yoshioka et al. 2022).

6.1.2 Benchmarking

For a reliable description of complex thermo-hydro-mechanical (THM) and reactive transport (RTP) processes, extensive tests of both the physical/chemical plausibility and the correct implementation in numerical simulators are essential. Figure 6.2 shows an sketch of benchmarks for THM/RTP models.

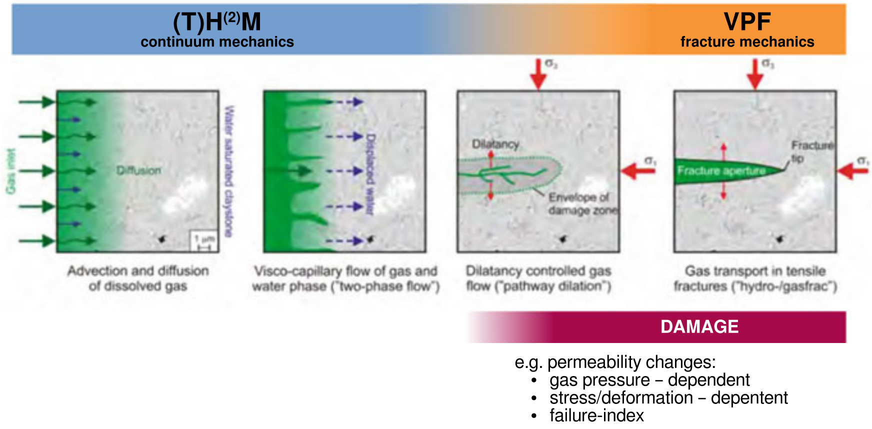

Fig. 6.1 Model chain for simulating consecutive processes of gas propagation in clay rocks leading to damage barrier integrity functions (Marschall et al. 2005), extended by Grunwald

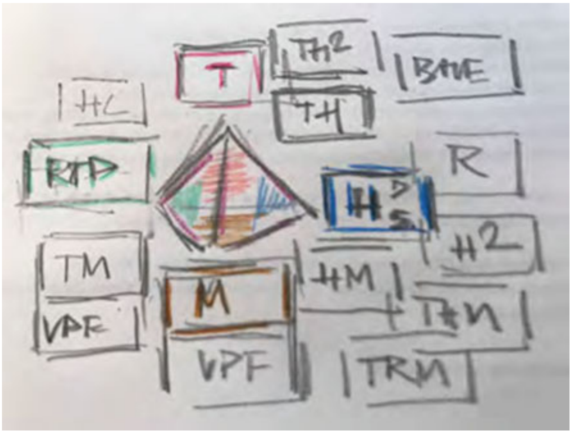

Fig. 6.2 Sketch of benchmark arrangement of THM/RTP models

An extensive suite of test examples was created for the development of the OGS-TH2M model (Grunwald et al. 2022). A hierarchical concept was developed and implemented that systematically checks all (reasonable) process couplings based on the individual processes (Fig. 6.3). The extensive collection of benchmarks (>100 tested test examples) from OGS is directly available via the portal and offers users an ideal introduction to THM/CB modelling. Some of the OGS benchmarks are already available as Jupyter notebooks (Sect. 5.3.2) and can thus be integrated into other Python applications with the corresponding advantages of user-specific data analysis.

The OGS-TH2M model, a new process class, developed by Grunwald et al. (2022). A comprehensive benchmarking has been conducted with the BenVaSim (Lux et al. 2021; Pitz et al. 2022) and DECOVALEX projects (Sect. 6.2.1).

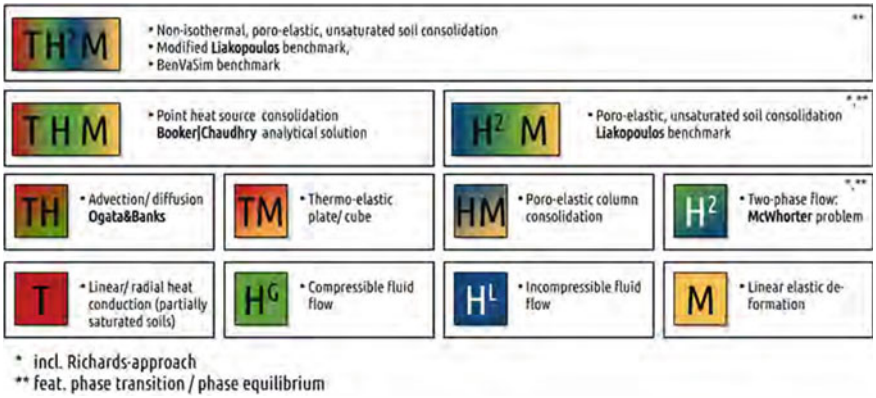

Fig. 6.3 Benchmarking hierarchy for TH2M processes (Grunwald et al. 2022)

6.2 International Collaboration

Fundamental developments from the GeomInt projects are widely used and deployed in various international collaboration activities in particular DECOVALEX, EURAD and the Mont Terri projects.

6.2.1 DECOVALEX

DECOVALEX (DEvelopment of COupled models and their VALidation against EXperiments) is an international research and model comparison project, initiated in 1992, for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological and geotechnical systems. DECOVALEX is an international community effort. OpenGeoSys is actively involved into all tasks of the current D2023 phase.[1] Task G is particularly dealing with the integrity of barrier rocks. This task is aiming to better understand reactivation of pre-existing discontinuities for brittle host rocks. In particular, the potential for existing features to undergo shear displacements and related changes in permeability as the result of coupled thermal, mechanical, hydraulic and chemical effects can all have significant impacts on repository safety functions (e.g., creating permeable pathways or, for very large displacements, mechanical damage of waste packages).

Task G is organised in four steps with increasing complexity (Fig. 6.4). The Task route starts from fracture mechanics (Step 1: M process) then diverting into hydro-mechanical (HM) and thermo-mechanical (TM) processes and finally combined into thermo-hydro-mechanical (THM) processes. These steps are described in the following including the concept, experimental design and data which will form

[1] https://decovalex.org/D-2023/overview.html.

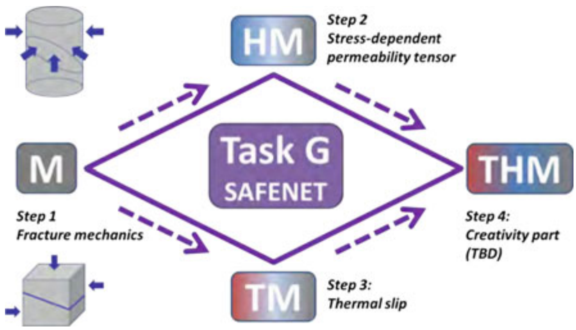

Fig. 6.4 Task G structure with related steps

the foundation for benchmarking exercises and experimental analysis. The research results are presented in the interim DECOVALEX report and the essence in Mollaali et al. (2022) which contains a comprehensive model and code comparison study including dis- and continuum mechanical approaches from all Task G members (nine international teams). Task G has been working on interpreting results from GeomInt laboratory experiments in Freiberg (Frühwirt et al. 2021) and Edinburgh (GREAT cell facility) (McDermott et al. 2018; Fraser-Harris et al. 2020).

6.2.2 EURAD

EURAD is a joint European project heading to safe radioactive waste management (RWM) through the development of a robust and sustained science, technology and knowledge management programme. It supports timely implementation of RWM activities and serves to foster mutual understanding and trust between Joint Programme participants.[2] GeomInt closely cooperated within EURAD particularly by contributing modeling know-how to work packages DONUT and GAS which are aiming at improving the understanding barrier integrity of clay formations in Europe suited as host rocks for deep geological repositories. GeomInt, therefore, actively helps in building European competences in clay systems understanding. Through EURAD national and international activities such as GeomInt, iCROSS, BenVaSim (Lux et al. 2021), DECOVALEX are bridged (Fig. 6.5).

6.3 Workflows—Mont Terri Project

One of GeomInt's main synthesis services is the development and implementation of workflows for the analysis of geotechnical systems. This is to be shown as an example for the joint work in the Mont Terri rock laboratory. Only the main features

[2] https://www.ejp-eurad.eu/.

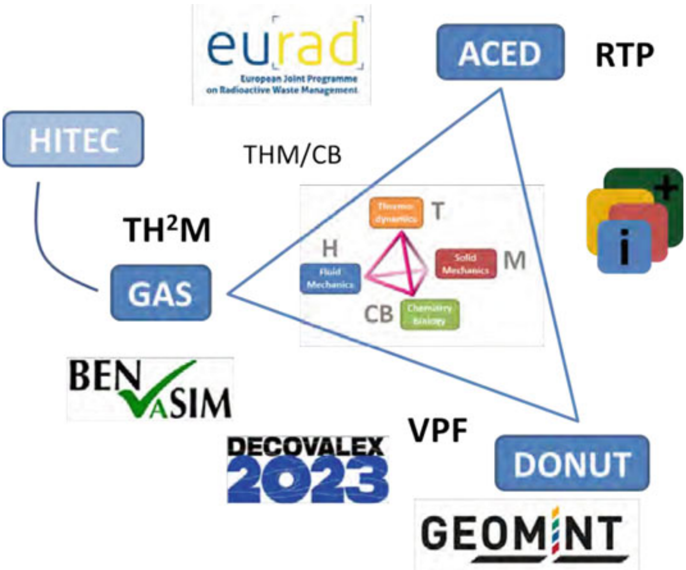

Fig. 6.5 International collaboration scheme—process-based cooperation for building European competences

of the workflow are shown here and the full description in Chap. 2 is referred to for details. (link Project geography)

The experimental basis is based on BGR field experiments in the Mont Terri rock laboratory and subsequent laboratory experiments. For example, drillcore samples were taken from the sandy facies of the OPA and analyzed in the geotechnical laboratory of the University of Kiel. The anisotropic, fracture and shrinkage behaviors were examined (observation/monitoring) in detail. The CD-A field experiment at Mont Terri has played a central role as a bridge between laboratory and field scales (ref). Much of the data from the URL Mont Terri was visually integrated into an information system as described in (ref) (Data Integration) The laboratory experiments (e.g. on the fracture behavior of the clay samples) were simulated using different model approaches. The essential processes and parameters that are relevant for the barrier integrity could be identified. (Process Simulation/Data Analytics) On this basis, a first transfer of the models to the field scale could be carried out. Exemplary, we were able to model cracks due to excavation and due to desiccation using discrete and diffuse approaches. In addition, an experimental design was carried out in advance for the planning of the CD-A experiment: the optimal distance between the two niches of the CD-A experiment was determined by numerical modeling and then implemented accordingly. This is an example of the use of models for the planning of complex and often expensive field experiments (Data Analytics/Knowledge Transfer). Finally, much of the experimental and modeled data and results have been integrated into the Visual Information System for Mont Terri and are available for

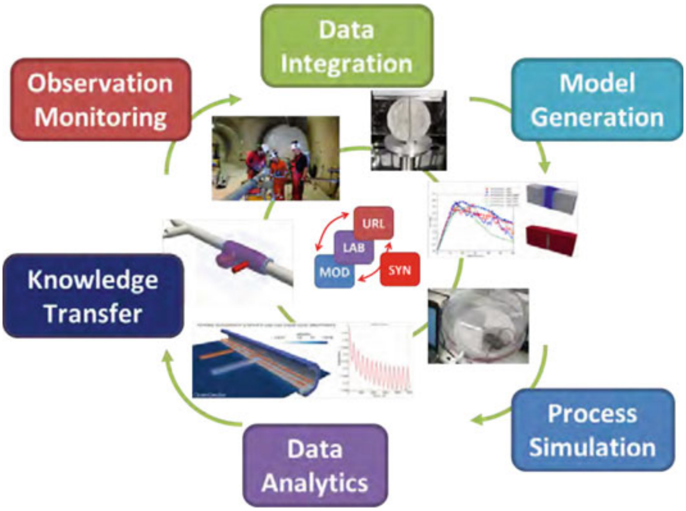

Fig. 6.6 Workflow concept applied to clay rock systems of the rock research laboratory in Mont Terri

various planning, discussion and demonstration purposes (knowledge transfer) (Fig. 6.6).

In addition to the CD-A experiment, currently more experiments from the Mont Terri rock laboratory are integrated into the workflow concept, e.g. the FE (full scale emplacement heater) and FS (fault slip) experiments targeting at the "proof-of-concept" for comprehensive workflows for entire research labs. The laboratory tests carried out in this phase of the GeomInt project, e.g. fluid percolation, will serve as basis for the application of numerical methods to model in the latter in-situ tests. Future work will be dedicated to further professionalize the workflow concept and transfer the know-how and software framework to other research labs.

References

Fraser-Harris, A., McDermott, C., Couples, G., Edlmann, K., Lightbody, A., Cartwright-Taylor, A., Kendrick, J., Brondolo, F., Fazio, M., & Sauter, M. (2020). Experimental investigation of hydraulic fracturing and stress sensitivity of fracture permeability under changing polyaxial stress conditions. *Journal of Geophysical Research: Solid Earth, 125*(12).

Frühwirt, T., Pötschke, D., & Konietzky, H. (2021). Simulation of direct shear tests using a forces on fracture surfaces (FFS) approach. *Environmental Earth Sciences, 80*(8).

Grunwald, N., Lehmann, C., Maßmann, J., Naumov, D., Kolditz, O., & Nagel, T. (2022). Non-isothermal two-phase flow in deformable porous media: Systematic open-source implementation and verification procedure. *Geomechanics and Geophysics for Geo-Energy and Geo-Resources, 8*(107).

Kolditz, O., Fischer, T., Frühwirt, T., Görke, U. -J., Helbig, C., Konietzky, H., Maßmann, J., Nest, M., Pötschke, D., Rink, K., Sattari, A., Schmidt, P., Steeb, H., Wuttke, F., Yoshioka, K., Vowinckel, B., Ziefle, G., & Nagel, T. (2021a). Geomint: geomechanical integrity of host and barrier rocks-experiments, models and analysis of discontinuities. *Environmental Earth Sciences, 80*(16).

Kolditz, O., Görke, U. -J., Konietzky, H., Maßmann, J., Nest, M., Steeb, H., Wuttke, F., & Nagel, T. (2021b). GeomInt – mechnanical integrity of host rocks. In *Terrestrial Environmental Sciences* (p. 277). Heidelberg: Springer.

Lux, K. -H., Rutenberg, M., Feierabend, J., Czaikowski, O., Friedenberg, L., & Maßmann, J. (2021). Benvasim - international benchmarking for verification and validation of THM simulators with special consideration of fluid dynamical processes in radioactive waste repository systems: Synthesis report: Reporting period: 01.05.2017-31.03.2021. Tech. Rep., Clauthal-Zellerfeld.

Marschall, P., Horseman, S., & Gimmi, T. (2005). Characterisation of gas transport properties of the Opalinus clay, a potential host rock formation for radioactive waste disposal. *Oil and Gas Science and Technology, 60*(1), 121–139.

McDermott, C., Fraser-Harris, A., Sauter, M., Couples, G., Edlmann, K., Kolditz, O., Lightbody, A., Somerville, J., & Wang, W. (2018). New experimental equipment recreating geo-reservoir conditions in large, fractured, porous samples to investigate coupled thermal, hydraulic and polyaxial stress processes. *Scientific Reports, 8*(1).

Mollaali, M., Kolditz, O., Mengsu, H., Park, C. -H., Park, J. -W., McDermott, C., Chittenden, N., Bond, A., Yoon, J., Zhou, J., Pan, P. -Z., Liu, H., Hou, W., Lei, H., Zhang, L., Nagel, T., Barsch, M., Wang, W., Nguyen, S., Kwon, S., Lee, C., & Yoshioka, K. (2022). Comparative verification of hydro-mechanical fracture behavior: Task G of international research project DECOVALEX 2023. *International Journal of Rock Mechanics and Mining Sciences*. Under review.

Pitz, M., Kaiser, S., Grunwald, N., Kumar, V., Buchwald, J., Wang, W., Naumov, D., Chaudhry, A., Maßmann, J., Thiedau, J., Kolditz, O., & Nagel, T. (2022). Non-isothermal consolidation: A systematic evaluation of two implementations based on multiphase and richards equations. *International Journal of Rock Mechanics and Mining Sciences*. Under review.

Yoshioka, K., Sattari, A., Nest, M., Günther, R. -M., Wuttke, F., Fischer, T., & Nagel, T. (2022). Numerical models of pressure-driven fluid percolation in rock salt: nucleation and propagation of flow pathways under variable stress conditions. *Environmental Earth Sciences, 81*(5).