CODE_BRIGHT
v9

VALIDATION DOCUMENT

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1 INTRODUCTION

The code has been extensively verified and validated in international benchmark exercises (DAM, EVEGAS, CATSIUS CLAY, BAMBUSII, MODEX REP, DECOVALEX). Patch tests and comparison with analytical solutions and other codes have been performed for each single equation (heat flow, gas and liquid flow in porous media, elastic and rigid plastic solution) and, when possible, for coupled problems (elastic consolidation, thermal convection in saturated porous media) (see for instance Olivella 1995; Alonso and Alcoverro 1999).

Validation by comparison with laboratory and field data has been realised in multiple THM problems related to nuclear waste storage in salt formations, stiff clays and expansive clays (Olivella et al. 1996; Gens et al., 1998; Alonso and Alcoverro 1999; Alonso et al., 2005; Rutqvist et al., 2005; Mata et al., 2006; Gens et al., 2007; Gens et al., 2009; Rodriguez-Dono et al., 2018; among others). Gas transport problems in clay barriers in laboratory and field scales have also been analysed (Delahaye et al., 2002; Alonso et al., 2006, Olivela & Alonso, 2008; Arnedo et al., 2008). The code has also been used to solve geotechnical problems such as rockfill embankments and drawdown in slopes and embankments (Alonso et. al., 2005; Pinyol, et. al., 2008).

Other validation examples and comparisons with measured data, in particular on the application of numerical formulations and advanced constitutive models have been published in international journals. Some examples to be highlighted are the numerical formulation for a coupled analysis of saline media (Olivella et al., 1994; Olivella et al., 1996); coupled solution of THM problems in saturated and unsaturated soils (Olivella & Gens, 2000; Saaltink et al., 2004; Chen at al., 2007); coupled THM and Chemical analysis in expansive clays (Guimaraes et al., 2007); constitutive models for crushed salt (Olivella & Gens, 2006), expansive materials (Sánchez et al., 2005) and frozen soils (Nishimura et al., 2009), among others.

The most relevant references of research projects and journal publications in which CODE_BRIGHT has been used are summarized in this document in a chronological way. A short description of some projects is also included. The compilation of references presented in this document, will be used as a further check on the performance of CODE_BRIGHT for the simulation of a wide range of engineering applications, provided that good quality material data and measurements of structural performance are available.

2 REFERENCES OF R+D PROJECTS (RAD-WASTE DISPOSAL)

This is a chronological list of research projects in the field of radioactive waste disposal related to CODE_BRIGHT use and development:

DAM project. Dam construction for the long term sealing of HLW repositories in salt formations. Project funded by the European Commission and ENRESA (RAD-WAS FI2W-CT90-0033, **1991-1995**).

CATSIUS CLAY project. Calculation and testing of behaviour of unsaturated clay as barrier in radioactive waste repositories. **Final report (1999). E.E. Alonso and J. Alcoverro.** Project forming part of the Research Programme on Nuclear Fission Safety of the European Commission (1996-1998). ENRESA. Publicación técnica Num. 10-11-12/99.

EVEGAS project. European validation exercise of gas migration models through geological media**. Final report (1997). Manai, T.** Project of the European Atomic Energy Community in the framework of its fourth R&D programme on Management and storage of radioactive waste. EUR 16639 EN (phase 1), EUR 17556 EN (phase 2) and 17557 EN (phase 3). Printed in Luxembourg.

PEGASUS project. Project on Effects of GAS in Underground Storage Facilities for Radioactive Waste. **Haijtink, B. and McMenamin, T. (Eds).** Commission of the European Communities. R&D programme on Management and Storage of Radioactive Waste. Proceedings of a progress meeting held in Brussels on 11-12 June/1992, EUR 14816 (**1993**). Proceedings of a progress meeting held in Köln (D) on June 3-4/1993, EUR 15734 (**1994**). Proceedings of a progress meeting held in Exeter (UK) on May 26-27/1994, EUR 16001 (**1995**). Proceedings of a progress meeting held in Rapolano Terme, Italy on 14-5 June/1995, EUR 16746 (**1996**).

BAMBUS project. Backfilling and Material Behaviour in Underground Salt Repositories. Phase I. **Final report**. Work performed as part of the European Atomic Energy Community's R&T Specific Programme Nuclear Fission Safety (**1994-1998**). Contract No. FI4W-CT95-0009. EUR 19124 EN.

PARCOMPWASTE project. A parallel computing solution for waste disposal problems and contaminant transport in the ground for use in an expert system for safety monitoring. Project funded by the European Commission (Copernicus), CP 94 0009 (**1996-1998**).

FEBEX Project. Full-Scale Engineered Barriers Experiment in Crystalline Host Rock. Project funded by the European Commission and ENRESA (1996-1999). **Final report, ENRESA 2000.** Publicación técnica (Empresa Nacional de Residuos Radiactivos (Espanya)); 1/2000.

BAMBUS II project. Backfilling and Sealing of Underground Repositories for Radioactive Waste in Salt, **Phase II**. **W. Bechthold, F.D. Hansen (Eds). Final report (2003).** Work performed as part of the European Atomic Energy Community's

R&T Specific Programme Nuclear Energy, key action Nuclear Fission Safety, 1998-2002 Area: Safety of the Fuel Cycle. EUR 20621.

DECOVALEX 3 Project. THM modelling of DST in situ test in Yuca Mountain. Project funded by the European Commission and ENRESA **(2000-2003**).

EB Project. Engineered Barrier Emplacement Experiment in Opalinus Clay for the Disposal of Radioactive Waste in Underground Repositories**. Final report (2005). J-C. Mayor, J-L. García-Siñeriz, E. Alonso, H-J. Alheid, P. Blümling.** Work performed as part of the European Atomic Energy Community's R&T Specific Programme "Nuclear Energy, Key Action: Nuclear Fission Safety 1998-2002" Area: Safety of the Fuel Cycle. EUR 21920.

VE Project. Ventilation Experiment in Opalinus Clay for the Disposal of Radioactive Waste in Underground Repositories. **Final report (2005). J.C. Major, J.L. García-Siñeriz, M. Velasco, J. Gómez-Hernández, A. Lloret, J-M. Matray,F. Coste, A. Giraud, T. Rothfuchs, P. Marschall, U. Roesli, G. Mayer.** Work performed as part of the European Atomic Energy Community's R&T Specific Programme "Nuclear Energy, Key Action: Nuclear Fission Safety 1998-2002" Area: Safety of the Fuel Cycle. EUR 21926.

Prototype Repository project. Full-Scale Testing of the KBS-3V Concept for the Geological Disposal of High-Level Radioactive Waste. **Final report (2005). C. Andersson, I. Bárcena, N. Bono, L. Boergesson, P. Cleall, T. Forsmark, D. Gunnarsson, L.-E. Johannesson, A. Ledesma, L. Liedtke, A. Luukkonen, K. Pedersen, I. Puigdomenech, R. Pusch, I. Rhén, T. Rothfuchs, T. Sandén, J.-L. Sineriz, Y. Sugita, C. Svemar, H. Thomas**. Work performed as part of the European Atomic Energy Community's R&T Specific Programme "Nuclear Energy, Key Action: Nuclear Fission Safety 1998-2002" Area: Safety of the Fuel Cycle. EUR 21924.

FEBEX Project. Full-Scale Engineered Barriers Experiment for a Deep Geological Repository for High-Level Waste in Crystalline Host Rock**. Updated Final report (1994-2004).** F. Huertas, P. Pariña, J. Farias, J.L. García-Siñériz, M.V. Villar, A.M. Fernández, P.L. Martín, F.J. Elorza, A. Gens, M. Sánchez, A. Lloret, J. Samper, M.A. Martínez. Publicación Técnica ENRESA 05-0/2006. 590pp, Madrid.

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HE Project. Heater Experiment: Rock and bentonite Thermo-Hydro-Mechanical (THM) processes in the near-field of a thermal source for development of deep underground high level radioactive waste repositories. **Final report (2006)**. Ingeborg

Göbel, Hans-Joachim Alheid, Norbert Jockwer, Juan Carlos Mayor, José Luis García-Siñeriz, Eduardo Alonso, Hanspeter Weber, Michael Ploetze, Georg Klubertanz, Christian Ammon Rothpletz. Work performed as part of the European Atomic Energy Community's R&T specific programme Nuclear Energy 1998-2002, key action Nuclear Fission Safety (Fifth Framework Programme) Area: Safety of the Fuel Cycle. EUR 22586.

MODEX-REP Project. Development of Hydro-mechanical Models of the Callovo-Oxfordian Argillites for the Geological Disposal of Radioactive Waste. **Final report (2007)**. **Edited by Kun Su**, Agence nationale pour la gestion des déchets radioactifs (Andra), FR. Work performed as part of the European Atomic Energy Community's R&T specific programme “Nuclear Energy 1998-2002, key action Nuclear Fission Safety” Area: Safety of the fuel cycle. EUR 20844.

NF-PRO Project. Understanding and Physical and Numerical Modelling of the Key Processes in the Near Field and their Coupling for Different Host Rocks and Repository Strategies (NF-PRO). **Final report (2008).** Project co-funded by the European Commission under the Euratom research and training programme on nuclear energy within the Sixth Framework Programme (2002-2006) Area: Management of radioactive waste. EUR 23730.

THERESA Project. Coupled thermal-hydrologycal-mechanical-chemical (THMC) processes for application in repository safety assessment. Project funded by the European Union, proposal/contract No. FP6-036458 (**2007-2009**).

FORGE project. Fate Of Repository GasEs. Project funded by the European Union, proposal/contract No. FP7- 230357 (**2009-2013**).

MUSTANG. CO2-MUSTANG is an EU project entitled: A MUltiple Space and Time scale approach for the quAntification of deep saliNe formations for CO2 storaGe (**2009 - 2013**).

DECOVALEX 2019. Participation in Task A to model gas injection tests.

2.1 Summary of some research projects

A brief description of some of the research projects is included in this chapter.

CATSIUS CLAY project

CATSIUS CLAY (acronym for Calculation and Testing of Behaviour of Unsaturated Clay as a Barrier in deep geological Radioactive Waste Repositories) was a Project forming part of the Research Programme on Nuclear Fission Safety of the European Commission. Its duration was from January 1st, 1996 to December 31st, 1998. The project aims at the verification and validation of available computer models capable of performing THM analyses. Seven modelling teams have been involved in this project respectively ANDRA(F), CLAY T.(SE), ISMES(IT), SCK-CEN(BE), UPC(ES), ULg(BE) and UWCC(GB). The project was co-ordinated by CIMNE, Barcelona, (E).

A total of six benchmark exercises were proposed to the modelling teams. These exercises were distributed in 3 stages: verification exercises, validation Exercises at Laboratory Scale and validation exercises at a large “in situ” scale. Two exercises were proposed at each stage. While the verification exercises had a more theoretical nature, the validation exercises dealt with phenomena taking place in engineered clayey barriers to be used in waste isolation. They address hydro-mechanical and thermo-hydro-mechanical problems under saturated and unsaturated conditions. Two exercises had a “blind” character. The codes used to solve the exercises were both commercial and in-house made codes. The first group include ABAQUS and PORFLOW while the second one includes CLEO, CODE BRIGHT, LAGAMINE and COMPASS.

Although the validation exercises were complex, performance of all modelling teams in all exercises was, in general, good. However, some modelling teams did not achieve fully satisfactory results in some cases. The report provides an assessment of the capabilities of the codes used and helps also to establish the state of the art in thermo-hydro-mechanical computations as applied to engineering barrier systems.

EVEGAS project

The EVEGAS benchmark project, set up by the European Commission, aims at the verification and the validation of numerical software for modelling two phase flow phenomena (water/gas) in low permeability porous media. In this project participated seven organizations respectively ANDRA(F), GRS (D), QuanticSci (formerly Intera) (UK), SCK/CEN (BE), SMC(UK), UPC (ES) and ENSMP-CIG (F). The project was coordinated by Geostock (F) with the technical assistance of Bertin (F). The used codes included TOUGH, ECLIPSE, PORFLOWM GENESYS, CODE-BRIGHT and SUNIDJ.
The project was organised in three phases: the analysis of the codes and treatment of a simple problem with analytical solution, the calculation of a few problems based on laboratory experiments and the modelling of a repository scenario.

PEGASUS project

PEGASUS (Project on Effects of GAS in Underground Storage Facilities for Radioactive Waste) was a project of the Commission of the European Communities, in the framework of the R&D programme on Management and Storage of Radioactive Waste (1992-1996). The project covers both theoretical and experimental studies on the processes of gas formation in waste packages and near-field and gas flow through engineered barriers and the surrounding host rocks. In the project were involved approximately 20 organisations and research institutes from seven Member States.

BAMBUS II project

The BAMBUS II project (Backfilling and Sealing of Underground Repositories for Radioactive Waste in Salt), was undertaken as a joint project by nine partners from five countries: FZK (DE, co-ordinator), BGR (DE), DBE (DE), G.3S (FR), GRS (DE), IfG (DE), NRG (NL), UPC (ES), and US DOE/CBFO (USA) between August 2000 and April 2003. The project was funded by the European Commission and the national governments and authorities.

The principal scientific objective of the project was to extend the basis for optimising repository design and construction and for predicting the long-term performance of the following barriers in a repository: (i) the host rock including the Excavation Disturbed Zone (EDZ) around emplacement rooms, (ii) the backfill (crushed salt), and (iii) the materials used for constructing durable waste containers. The work was divided into in situ studies, laboratory investigations, modelling studies, and desk studies. UPC participated in the THM modelling studies.

In situ investigations were carried out in the Asse salt mine subsequent to completion of the large-scale TSDE (Thermal Simulation of Drift Emplacement) in which two simulated emplacement drifts had been electrically heated to between 170 and 200 °C by disposal cask mock-ups over more than eight years. In one drift, backfill, two heaters, and measuring instruments were recovered. Local conditions in backfill and surrounding rock were examined and samples of native salt and consolidated backfill were studied in laboratories. Instruments were retrieved for analysis of their performance during the experiment execution and for recalibration. Extensive geophysical studies characterized the development of the EDZ around excavations.

Laboratory tests measured properties of specimens extracted from the backfill in the dismantled drift as well as cores from the surrounding rock. Physical, mechanical, and hydrological experiments quantified parameter values requisite for material models and described attributes of backfill and rock salt at advanced stages of compaction and deformation. An extensive array of 280 candidate container material samples was recovered and examined to evaluate their state of corrosion, which was minimal after more than ten years of exposure in the TSDE experiment.

A suite of modelling studies analysed the thermo-mechanical evolution of the TSDE and evaluated the predictive capabilities available to address complex modelling demands associated with long-term repository predictions. These computational studies helped to refine models and codes based on forensic investigations in the dismantled experimental drift and from laboratory tests. Advancements recognized in

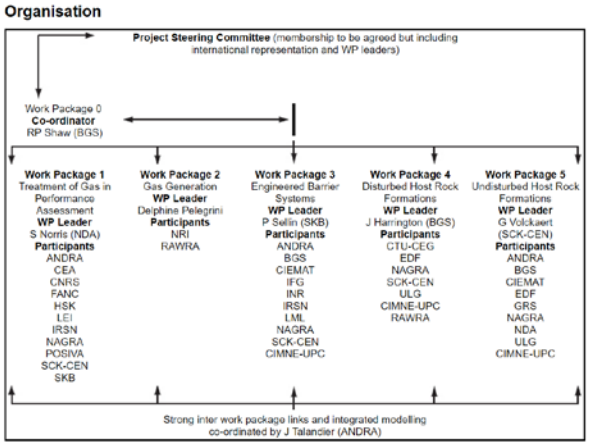
a breadth of applications improved comparisons between computational results and in situ experimental results from the TSDE. Post-test investigations served to reconcile lingering differences between experiments and calculations witnessed at the conclusion of the BAMBUS-I project. The primary results encompass comprehensive computational approaches that demonstrate successful prediction of temperature profiles, stress distributions, displacements, and the attendant properties of compacted backfill, intact rock salt and the EDZ.

In a desk study the boundary conditions for the retrievability of highly active waste and spent fuel were investigated. The consequences of the accessibility of the waste during the retrievability period were assessed. In addition, the technical and scientific results of the TSDE project (1985 to 2002) were reviewed and documented. For use in future repository design and construction, an easily accessible data acquisition system was developed.

FORGE project

Fate Of Repository Gases

Long-term radioactive waste management usually considers final disposal in a deep geological repository. This includes an engineered barrier system working in conjunction with the surrounding host rocks to minimise migration of radioactivity. As the repository system evolves, gases may be produced, such as hydrogen from the corrosion of metals and from the radiolysis of water, and radon from the radioactive decay of some of the waste. If present, biodegradable wastes can also produce carbon dioxide and methane. Understanding how these gases move in a repository setting is a topic identified for further study. The FORGE project, which ran from February 2009 to September 2013, studied key gas migration issues in repository performance assessment.



CIMNE participation in WorkPackages 3, 4 and 5 lead to participation in several modelling exercises including gas flow modelling in EDZ, clay barriers and argillite. Corresponding publications by Arnedo et al (2013) and Alcoverro et al (2014) are included in the publication section.

MUSTANG

CO2-MUSTANG is an EU project entitled: A MUltiple Space and Time scale approach for the quAntification of deep saliNe formations for CO2 storaGe.

MUSTANG is a four year large-scale integrating project to span from 2009 to 2013 and to be funded by the EU FP7, under the coordination of the Uppsala University. The MUSTANG consortium comprises 19 institutions. It aims at developing guidelines, methods and tools for the characterization of deep saline aquifers for long term storage of CO2, based on a solid scientific understanding of the underlying critical processes. Field investigation technologies specifically suited to CO2 storage will be improved and developed. These are destined to improve the determination of the relevant physical and chemical properties of the site, and enabling short response times in the detection and monitoring of CO2 plumes in the reservoir and overburden during both the injection and containment phases. An improved understanding of the relevant processes of CO2 spreading is aimed at by means of theoretical investigations, laboratory experiments, natural analogue studies as well as a dedicated field scale injection test, to take place at the Heletz site (Israel).

CODE_BRIGHT was used by modelling team at CSIC and UPC. Publications by Vilarrasa et al can be found at the publication list in this document.

This project was a great opportunity to widen the capabilities of CODE_BRIGHT. Implementation of equations of state (EOS) for CO2 was the starting point in this project. In an early stage, hydro-mechanical calculations permitted to study the effect of carbon injection on ground surface uplift and earthquake induction. As a continuation, non-isothermal modelling permitted to investigate along the different states of carbon at the point of injection and penetration into deep aquifers. It was proposed to inject Liquid CO2 instead of in a Supercritical state. The later was more or less an assumed condition but the results of the project show that it is perhaps only one possibility.

DECOVALEX
modElliNg Gas INjection ExpERiments (ENGINEER)

In a geological repository for radioactive waste, the corrosion of the ferrous materials, radioactive decay of the waste, radiolysis of organic materials and water, and the microbial breakdown of organic materials will produce gas, the most important of which (by volume) is hydrogen. Depending on the repository concept, the production of these gases may span in excess of 100,000 years, following emplacement of the waste. As gas is produced, it will accumulate, moving away from its source through the combined processes of molecular diffusion and bulk advection. Understanding these processes, the long-term fate of the gas and its impact on the surrounding materials is therefore important in the development of a geological disposal facility (GDF) for radioactive waste.

The purpose of Task A in DECOVALEX-2019 is to better understand the processes governing the advective movement of gas in two low permeability materials: (i) one engineered (compacted bentonite) and (ii) one a potential, natural repository host rock

(in this case the Callovo Oxfordian Claystone). Special attention is given to the mechanisms controlling factors such as gas entry and flow, as well as pathway stability and sealing, which will impact barrier performance. To underpin this task, new numerical representations for the quantitative prediction of gas fluxes will be developed. These will be tested against a series of controlled laboratory tests, in a staged manner, building in complexity (both in terms of the experimental and modelling approaches). It is anticipated that the development of these models will provide a valuable tool to assess the impact of gas flow on barrier and host materials, providing information which could be used to support future repository design.

In addition, experience gained through this task is of direct relevance to other clay-based engineering issues where advective gas flow is involved, including: shale gas, hydrocarbon migration, carbon capture and storage, gas storage and landfill design.

3 REFERENCES OF JOURNAL PUBLICATIONS

Publications are included in this chapter in chronological order.

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