Modeling of Coupled Thermo-Hydro-Mechanical-Chemical Processes for High-Level Radioactive Waste Repositories–17361

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ABSTRACT
To ensure that multibarrier systems in high-level radioactive waste (HLW) repositories can efficiently perform their functions and isolate the waste from the biosphere, coupled thermo-hydro-mechanical-chemical (THMC) processes used for the performance assessment of HLW disposal facilities should be modeled. To evaluate coupled THMC processes, the DECOVALEX project, a unique international research collaboration project initiated in 1992, developed mathematical models and field experiments involving THMC processes in engineered barrier systems and host rocks for HLW disposal. The DECOVALEX project and the current status of coupled THMC model development can provide further insights into the performance assessment of HLW disposal facilities. This study provides information regarding the DECOVALEX project and reviews the development of coupled THMC models. The study results furnish knowledge of coupled THMC processes and techniques for the performance assessment and safety analysis of the final HLW disposal.

INTRODUCTION
The International Atomic Energy Agency recommends that high-level radioactive waste (HLW) be buried in subterranean formations, approximately 300–1000 m deep, by using the isolation and segregation characteristics of deep rock formations in natural barriers while engineering geological disposal systems. The multibarrier systems can encapsulate, isolate, or delay various nuclear hazardous contaminants and ensure the reliable, long-term performance of disposal facilities. It also prevents adverse effects on human health and the environment [1-2]. Witherspoon [3-5] reported that a multibarrier system comprises an engineered barrier, composed of waste form, waste package, buffer or backfill material, and the natural barrier, formed by the host rock. Crucially, it ensures that radioactive waste decay remains harmless to the biosphere.

The properties of the final disposal site are as follows: very low permeability, high thermal conductivity, absence of a crustal structure or volcanic activity, absence of natural resources in the vicinity, self-sealing lithology, high strength, visco-plastic (creep) deformation behavior of rock salt, isotropic static stable state of the rock with high adsorption, reliable stability at a high temperature, low water content, and low lithological variability [2, 6]. When a crystalline rock is selected as the host rock, bentonite is mostly used as the buffer or backfill material for multibarrier systems at disposal sites. The buffer material should have high thermal conductivity so that the decay heat, generated from the waste package, can be effectively conducted to the host rock, the near-field heat load can be reduced, and the temperature can be prevented from exceeding 100°C. The thermal conductivity of the buffer material can inhibit the effect of buffer material degradation and maintain the original saturation state because of water vaporization. To prevent degradation caused by decay heat and the load of the waste package, the buffer material should retain its physical, chemical, and mineral properties for long-term stability. The disposal site exhibits naturally existing cracks, excavation damage zones, or cracks formed by the heat generated by the nuclide transport pathway. Hence, the ideal buffer material must have micro shrinkage characteristics and not drying shrinkage, which results in the formation of cracks [7]. Bentonite as a buffer material in HLW disposal is a crucial engineered barrier. The buffer material is situated between the radioactive waste containers and the surrounding host rock. Additionally, bentonite is in direct contact with the decay heat of radioactive waste, stress around the host rock, groundwater flow, and chemical species under the influence of such thermo-hydro-mechanical-chemical (THMC) effects. Therefore, investigating the complex THMC coupling can provide further insights into the performance assessment of buffer materials for the long-term safety analysis of radioactive waste disposal sites.

DECOVALEX THMC STUDY

Initiated in 1992, DECOVALEX (DEvelopment of COupled models and their VALidation against EXperiments in nuclear waste isolation) was proposed by Sweden, and major nuclear energy countries cooperated in this project. Ten countries, including the United States, France, the United Kingdom, Germany, Japan, Canada, Sweden, and Finland, and 15 research institutions have been involved in the project since it was initiated. The project developed the algorithm for the thermal-hydro-mechanical (THM) scheme and model. The study results were compared with field and laboratory data, and then new experiments were designed to validate the model. THM is also used to analyze the performance assessment of disposal safety. DECOVALEX research is divided into two categories. The first is the benchmark test (BMT), wherein a THM scenario is assumed to compare the calculation results between the mathematical scheme and the developed code model. The second is the test case (TC), which is an in situ experiment to confirm the reliability of the developed model. The implementation of DECOVALEX was originally planned in four phases. During the first three phases, several codes (MOTIF [8], THAMES [9], ADINA-T [10], ROCMAS [11], CHEF [12], HYDREF [12], VIPLEF [12], TRIO-EF [13], CASTEM2000 [14], and UDEC [15]) were developed in discrete and continuous methods. Coupling problems involving two processes (such as HC, TH, and HM) and three processes (such as THC and THM) were developed. In the fourth phase, the chemical process (C) was included in the complete process, which was then further integrated into the THMC complete coupling process by using the HMC or THC coupling processes as the main research content [16-17]. However, DECOVALEX-2011 (2008–2011) and DECOVALEX-2015 (2012–2015) were implemented after the completion of DECOVALEX IV in 2007.
The results of the four phases are summarized in Table I [17-18], and more detailed information can be found in the literature [17-33].

TABLE I. Phases, tasks, and results of the DECOVALEX I–IV projects.

Phase or time period	Benchmark test (BMT), test case (TC), and task	References
DECOVALEX I,	BMT 1:(THM coupling) Two orthogonal sets of persistent fractures and a heat	Book: *Coupled T-H-M processes of fractured*

Phase or time period	Benchmark test (BMT), test case (TC), and task	References
1992–1995	source in a fractured rock, 3000 × 1000 m^2 in size, two-dimensional far field. BMT 2: (THM coupling) Four discrete fractures and a finite length heat source in a fractured rock, 0.75 × 0.5 m^2 in size, two-dimensional near field. BMT 3: (THM coupling) A realistic fracture network of 6,580 fractures from Stripa mine data in a fractured rock, 50 × 50 m^2 in size, two-dimensional near field. TC 1: (THM coupling) Laboratory shear-flow test on a rock core sample with a single joint, 260 x 260 mm^2 in size, two-dimensional problem. TC 2: (THM coupling) Field experiment in a fractured rock at Fanay-Augères, France, 10 × 10 × 5 m^3 in size, three-dimensional problem. TC 3: (THM coupling) Large-scale laboratory experiment of engineered buffer material (Big-Ben experiment, Japan). TC 4: (MC coupling) Axial normal stress flow coupling process in a fractured rock mass. TC 5: (MC coupling) Shear-flow coupling test for a single joint in a fractured rock, two-dimensional problem. TC 6: Field experiment of a hydraulic injection test on fractures at a depth of 356 m.	*media* (27 papers) [25] Special issue of *Int J Rock Mech Min Sci Geomech Abstr* vol 32 No.5, 1995 (9 papers) [26]
DECOVALEX II, 1995–2000	Task 1: Numerical simulation of Nirex's Rock Characterization Facility shaft excavation at Sellafield, United Kingdom. Task 2: In situ THM coupling test and numerical simulation of the host rock properties of the underground heating laboratory in Kamaishi Mine, Japan. Task 3: Study on the constitutive relations of rock joints.	Special issue of *Int J Rock Mech Min Sci* vol 38 No.1, 2001 (12 papers) [27]

Phase or time period	Benchmark test (BMT), test case (TC), and task	References
	Task 4: Study on THM coupling processes for design and safety assessment of radioactive waste disposal sites.	
DECOVALEX III, 2000–2003	Task 1: FEBEX (Full-scale engineered experiments in crystalline host rock) underground laboratory heating test for ENRESA in Grimsel mine, Switzerland. Task 2: The drift scale test at Yucca Mountain, United States. BMT 1: Implication of THM coupling in near-field safety of radioactive waste disposal. BMT 2: Upscaling of the THM properties in a fractured rock mass and its significance for large-scale repository PA. BMT 3: The THM responses to a glaciation cycle and their potential implications for deep geological disposal of nuclear fuel waste in a fractured crystalline rock mass.	Proceedings GeoProc 2003; Coupled T-H-M-C processes in geosystems (Stephansson et al. 2004) (33 papers) [28] Special issue of *Int J Rock Mech Min Sci* vol 42 No. 5–6, 2005 (18 papers) [29]
DECOVALEX IV, 2004 – 2007	Task A: (THM coupling) Near-field effects on functional safety of spent nuclear fuel disposal sites. Task B: (HMC coupling) Study on HMC coupling of crystallized rock in excavation damaged zone (EDZ). Task C: (HM coupling) Simulation of EDZ in the argillaceous Tournemire Field of Mudstone excavation in France. Task D: Long-term permeability or porosity changes in the EDZ and near field because of THM and THC processes in volcanic and crystalline–bentonite systems. Task E: (THM coupling)THM processes associated with long-term climate change: glaciation case study.	Proceedings GeoProc 2006 (24 papers) [30] and *Special issue of Environ Geol* (12 papers) [31]

DECOVALEX-2011 (2008–2011)

Funding organizations from nine countries, namely Sweden, the United States, Canada, the Czech Republic, France, Japan, Korea, Spain, and China, supported DECOVALEX-2011. The topics included the effects of radioactive waste disposal facilities on the stability of the host rock, groundwater flow, and solute transport in the host rock during the excavation and construction periods. The focus of DECOVALEX-2011 was assessing the effect of THMC coupling processes on the safety of disposal facilities. The full-scale engineering model data compared these effects between Switzerland, Sweden, and other underground research laboratories on the basis of the results from these laboratories. The model was divided into three tasks, A, B, and C, as follows: [23, 32]

Task A: Hydro-mechanical (HM) coupling and chemical (C) variation in argillaceous rock. The HM coupling effect of argillaceous rock fissures and the host rock under ventilation conditions and the chemical reaction were examined. Additionally, the sensitivity of the argillaceous rocks during saturation, dehydration, and rewetting cycles, as well as the hydro-chemical (HC) influence on the damage zone, was investigated. [23, 32]

Task B: Thermo-mechanical coupling simulation of mechanical effects and failure characteristics of the rock mass during excavation, and the temperature rise between adjacent disposal holes, were examined. Sweden established a large-scale underground test of Äspö Pillar Stability Experiment (APSE) in the host rock of granite. The main purpose of the experiment was to study the failure process of heterogeneous rock under the condition of coupled stress and temperature. The horizontal test well was 450 m deep, 80 m long, 5 m wide, and 7.5 m high with an axis at N46° E. [23, 32-33]

Task C: THMC coupling and assessment for single fractured and fractured rock masses. The TC focused on the hydrogeological problem at the Bedrichov tunnel site in the Czech Republic, and included data collection and model construction as well as parameterization and uncertainty analysis for the groundwater flow simulation and tracer test transport processes. A simulation experiment was conducted on the complex fracture network model and the distribution of the velocity field of the fracture network in a single fissure of granite in Beishan, China. [23, 32]

DECOVALEX-2015（2012–2015）

Ten international research institutes participated in five tasks to conduct complex field and laboratory tests in Switzerland, France, Japan, and the Czech Republic. In particular, DECOVALEX-2015 focused on the THMC coupling behavior for multibarrier systems (comprising engineered and natural barriers) of host rocks in argillaceous and crystalline rocks. [23]

Task A: These experiments focused on the technical feasibility of the tunnel and shaft seals with respect to their safety functions and expected performance levels. The key issue pertained to the long-term performance of seal systems composed of bentonite (MX80 bentonite). Thus, Task A was based on a TC, the SEALEX project, which was conducted at the Tournemire underground laboratory in France by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN). The participating groups were the IRSN, France; the Canadian Nuclear Safety Commission, Canada; Institute of Geonics AS CR, Czech Republic; Quintessa and the University of Edinburgh and Imperial College, United Kingdom; and the Nuclear Regulatory Commission, United States. In the operational phase, water is first pumped into the injection chambers to saturate the clay core slowly through the injection lines connected to the injection chambers. The experimental design layout is illustrated in Figure 2. [23]

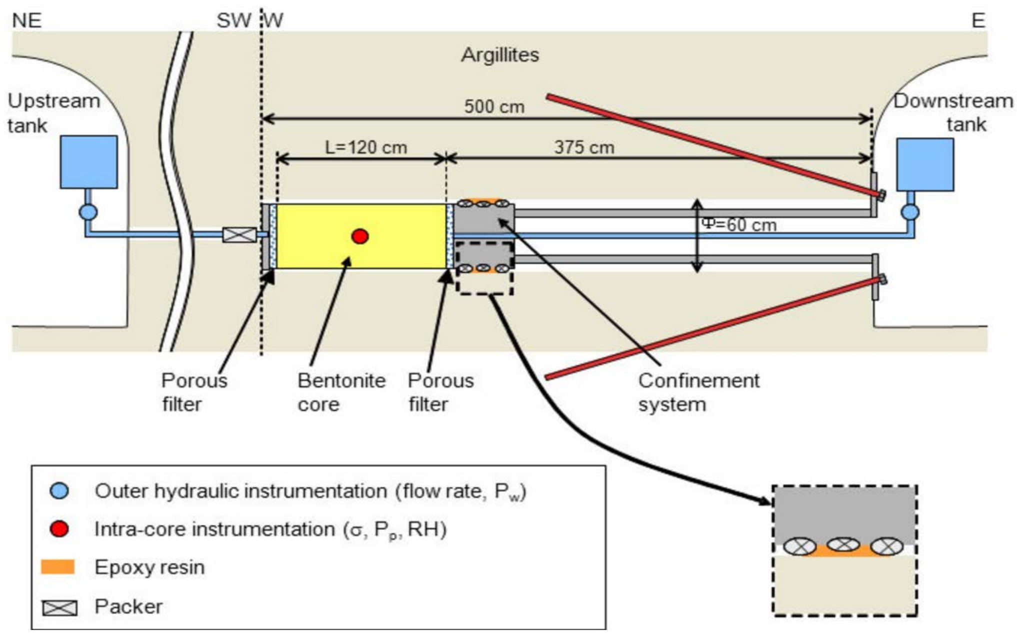

Fig. 1. Layout of the SEALEX in situ experiment.

Task B.1: Heating experiment (HE) for understanding the THM processes in a bentonite buffer and argillaceous host rock. This experiment is comprised of: (1) the HE-D in situ heating test (rock only), (2) laboratory column tests on bentonite pellets, and (3) the HE-E in situ heating experiment (integrating buffer materials and host rocks). The two in situ experiments were performed at the international Mont Terri rock laboratory in Switzerland. Figure 2 depicts the experimental design layout. [23]

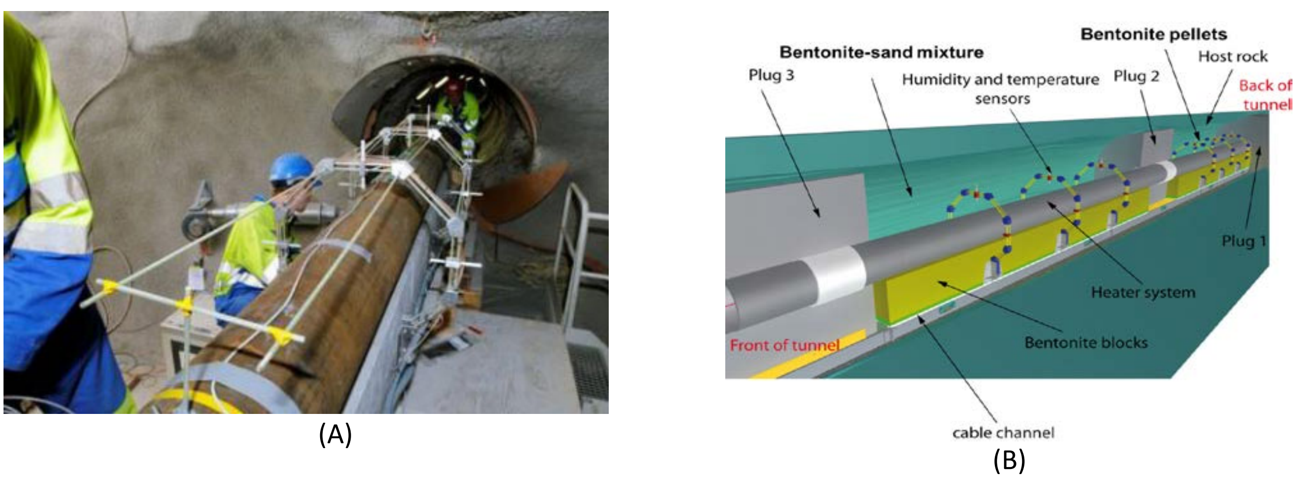

Fig. 2. HE-E heating experiment. (A) Installation of an HE-E Heater Test; (B) Schematic illustration of the experiment design in situ.

Task B.2: Coupled THM (or THMC) processes in the full-scale in situ engineered barrier system (EBS) experiment were conducted at the Horonobe underground research laboratory in Japan. The purpose of this experiment was to verify the safety of the EBS concept for the HLW (vitrified waste) in a sedimentary rock supported by a concrete lining. In the underground tunnel test, the electric heater denoted the decay heat source of HLW, surrounded by bentonite buffer material. The participating countries (research organization) included China (CAS), Germany (BGR), Japan (JAEA), South Korea (KAERI), and the United States (DOE). The experimental design layout is illustrated in Figure 3. [23]

Task C.1: Coupled THMC processes within single fractures were examined through the construction of appropriate mathematical models that were constrained by two sets of laboratory experiments. The experimental design was as follows: (1) coupled THMC process in homogeneous novaculite (quartz) and granite, (2) mechanical loading and variable temperature control conducted by pressurized water flow through artificial fracture cracks, and (3) chemical analysis for the effluent chemical species. Participating countries (research organization) included Germany (BGR), China (CAS), the Czech Republic (Czech Technical University of Liberec), the United Kingdom (NDA RWMD), and the United States (NRC). The experimental design layout is illustrated in Figure 4. [23]

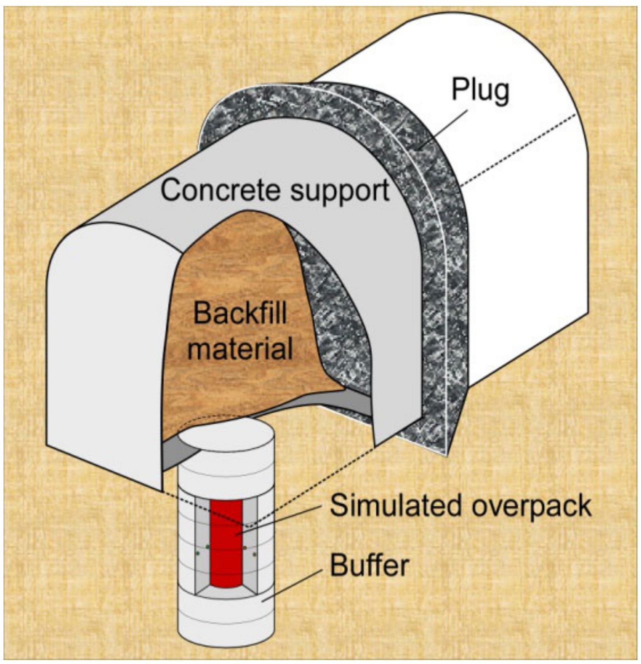

Fig. 3. Horonobe EBS experiment.

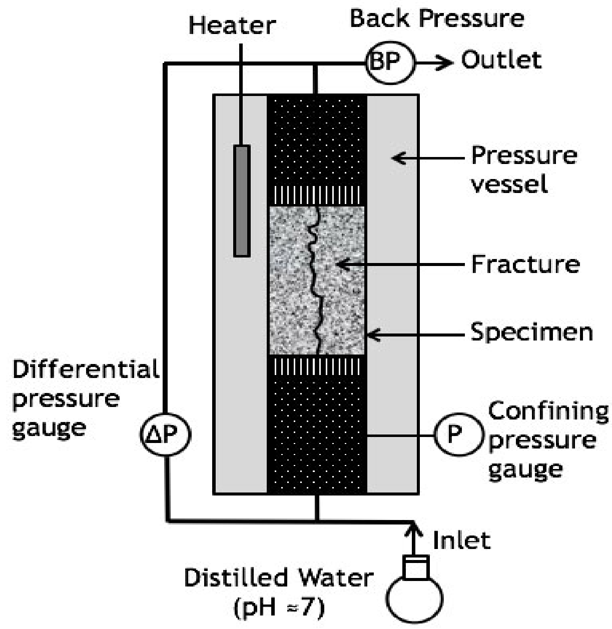

Fig. 4. Experimental design of THMC processes in single fracture plane.

Task C.2: Investigation of the groundwater flow, tracer transport, and reactive chemical transport in granite fissures of the Bedrichov tunnel, Czech Republic. The main issue was the inhomogeneity of the water flow, that is, the heterogeneous distribution of water, which results from differences in the size and scale of conduits (because of faults and fractures), and the relation of water quantity and flow velocity (or residence time). Furthermore, the uncertainty evaluation from calibration and blind prediction steps with partial data sequences, and from cross-validation with different models and data (hydraulics, tracers, and reactions), were performed. Participating countries (research organization) included the Czech Republic (RAWRA), Germany (BGR), and the United States (DOE Sandia National Laboratory). The experimental design layout is portrayed in Figure 5. [23]

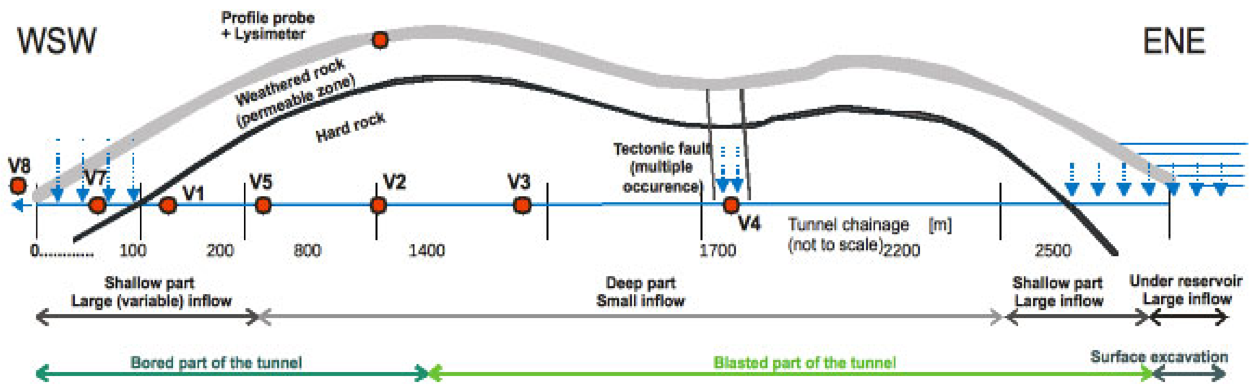

Fig. 5. Experimental design of the Bedrichov tunnel test.

For over 20 years, the DECOVALEX project has played a key role in the development of coupled THMC processes for the performance assessment of radioactive waste disposal repositories. The underground research laboratory obtains a large amount of scientific data, including the hydrogeological parameters of radionuclide migration (hydraulic conductivity coefficients and diffusion coefficients), and the THMC coupling parameters of EBS and natural barriers in host rocks, such as granite, argillaceous, tuff, and salt rock. The in situ experimental tests in fractured rock masses and the full-scale engineered barriers achieved the field verification of new and sophisticated coupled THMC models in EBS and fractured rock masses.

THMC COUPLING MODELING

Keyes et al. [34] provided a complete discussion of the recent innovations in multiphysics and multifunctional interdisciplinary software, with user-defined mathematical equations and extended model functional flexibility. The software contains user-generated, nonlinear partial differential equations (PDEs) and multiple algebraic equations that can be solved. Examples of the software include PETSC [35], MUSE [36], OOFEM [37], Chombo [38], Fenics [39] and COMSOL Multiphysics [40]. Notably, because COMSOL Multiphysics has a graphical interface with user-defined, nonlinear PDEs and multiple algebraic equations, it is able to establish complete engineering program modules and algorithms.

The geochemical model of PHREEQC [41] has been rewritten in C++ programming language and has modularized the PHREEQC model (called IPHREEQC) [42]. The IPHREEQC software incorporates a library of mathematical algorithms (similar to PHREEQC) and includes a complete chemical thermodynamics database accessible via an external numerical program library. The thermodynamics databases of WATEQ4F, MINTEQ, and EQ3/6 are also included [41, 43] in PHREEQC. The IPHREEQC link library has been successfully coupled with the COMSOL model through the code written in MATLAB [44]; for instance, the COMSOL–IPHREEQC model [45], coupled thermal-hydraulic-chemical-geomechanical model [46], THM-GeoC [47], and interface COMSOL–PHREEQC (iCP) [48] are available. Table II summarizes the development results of these relevant models [48].

The THMC model of COMSOL–IPHREEQC, THM-GeoC, and the iCP were developed by the DECOVALEX project for the performance assessment of HLW disposal. Notably, the COMSOL code was initially the PDE toolbox of the MATLAB module. Later, MATLAB was excluded and the module was renamed COMSOL Multiphysics; now, this module can solve PDEs in various multiphysics fields. The subsurface flow module of COMSOL Multiphysics contains fluid flow, heat transfer, and solute transport models and can simulate radioactive species migration in the repository. The waste form canister is ruptured by the external stress, and radionuclides are released from the waste container into the far field. To develop a COMSOL–IPHREEQC-coupled THMC model, we first attempted to simulate the radioactive nuclide release from the EBS using the COMSOL three-dimensional transport model. The configuration conditions included the groundwater flow conditions (velocity, direction, porosity coefficient, and diffusion coefficient), temperature conditions of waste decay heat, and physical properties of host rocks and EBS.

Table II. Model introduction of developed partially- or completely-coupled THMC processes since 1998

Code name	Developer	Physical and chemical processes included in the code				
		Heat transfer	Flow	Mechanical processes	Solute transport	Chemical reaction
		(T)	(H)	(M)	(C)	
HP1 HYDRUS1D-PHREEQC	Jacques and Šimůnek (2005) [49]		V		V	V
MIN3P	Mayer (2000) [50]		V		V	V
MT3DMS	Zheng and Wang (1998) [51]		V		V	
PHREEQC	Parkhurst and Appelo (1999) [41]		V		V	V
TOUGH-FLAC	Rutqvist and Tsang (2003) [52]	V	V	V		
TOUGHREACT	Xu et al. (2006) [53]	V	V		V	V
3DHYDROGEOCHEM	Cheng and Yeh (1998) [54]	V	V		V	V
COMSOL–IPHREEQC	Wissmeier and Barry (2011) [45]		V		V	V
FLAC3D-TOUGHREACT	Taron et al. (2009) [55]	V	V	V	V	V
THM-GeoC	Nasir et al. (2014) [47]	V	V	V	V	V
Coupled THCG Model	Seetharam and Jacques (2013) [46]	V	V	V	V	V
Interface COMSOL–PHREEQC(iCP)	Nardi et al. (2014) [48]	V	V	V	V	V

In this study, the SKB KBS-3 conceptual model was used to design the TC. The nuclide in the radioactive waste container will be slowly released into the buffer material. Because the hydraulic conductivity coefficient of the buffer material and the effective diffusion coefficient of the nuclide in the buffer material are already very low, after 100 years of release time, the concentration of the radioactive nuclide in the buffer material will remain very low. In 1000 years, the radioactive nuclide will be slowly deposited around the buffer material. Because the fracture fission of the host rock is assumed to be in the fully permeable state, the nuclide will slowly be transported to the backfill material (the disposal tunnel) over time. Although the boundary on the right side of the backfill material is set to the open outflow boundary, the radioactive nuclide will not flow out to the boundary within the simulation time of 10,000 or 100,000 years. The diffusion of nuclide is the dominant transport mechanism through the buffer and backfill materials (Figures 6 and 7).

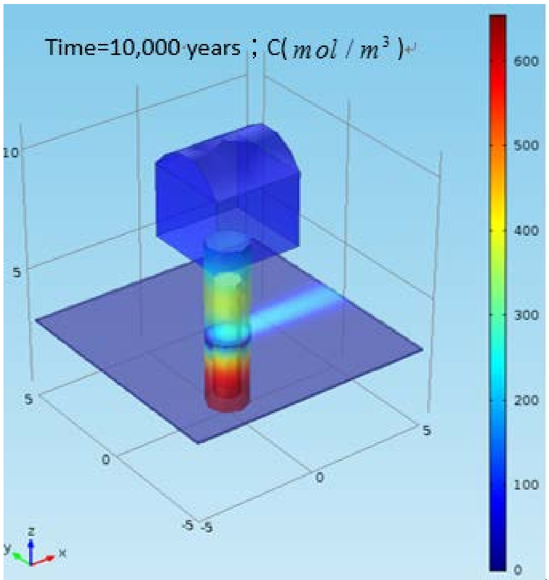

Fig. 6. Three-dimensional transport of a THMC-coupled model analysis for HLW disposal over 10,000 years.

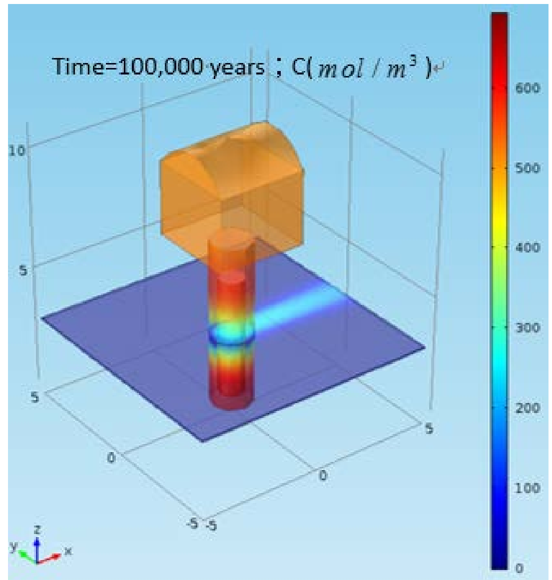

Fig. 7. Three-dimensional transport of a THMC-coupled model analysis for HLW disposal over 100,000 years.

DISCUSSION

The DECOVALEX project has made numerous crucial comments related to THMC-coupled processes, as well as significant progress in the development of numerically modeled coupled processes in fractured rocks and buffer and backfill materials. This study presented an overview of the DECOVALEX project and the use of the DECOVALEX development model. In the future, we will apply the knowledge gained from the DECOVALEX project to develop the feature, event, and process of THMC coupling using the COMSOL and PHREEQC geochemical models to support the performance assessment of HLW disposal in Taiwan.

The COMSOL module is a finite element modeling program used to solve a wide range of PDEs with applications for the performance assessment of the HLW disposal repository. Flexibility within the software allows users to couple multiple PDEs within a single model domain (e.g., variably saturated ground water flow with heat transport), as well as couple multiphysical problems within adjoining model domains (e.g., ground water flow coupled with solute transport, heat transfer, geomechanics, and chemical reactions). COMSOL contains a basic library of predefined PDEs for specific applications (e.g., convection or diffusion, fluid dynamics, and heat transfer) and generalized PDEs that can be adapted for specific problems [40, 56]. Moreover, the COMSOL module can support a live link with the MATLAB program. Various algorithms are capable of coupling the COMSOL and MATLAB modules; notably, this software feature can then also facilitate the coupling of the COMSOL and IPHREEQC modules.

CONCLUSIONS

Advancing the understanding and mathematical modeling of coupled THMC processes in the EBS of HLW disposal facilities and geological systems is required for the performance assessment of HLW disposal repositories. However, studies regarding THMC processes in the host rocks affected by the excavation and heat production by the radionuclide decay in radioactive waste have not been conducted in Taiwan. The primary focus in Taiwan was on individual phenomena, such as thermal, hydraulic, mechanical, and chemical processes, or coupled T-M issues associated with a radioactive waste repository. To evaluate the coupled THMC processes, the DECOVALEX project, a unique international research collaboration, has been implemented since 1992 to develop mathematical models and field experiments for THMC processes in EBS and repository host rocks for HLW disposal. The DECOVALEX project results, and the current status of coupled THMC for disposal facilities of spent nuclear fuel, can provide further THMC insights into HLW disposal in Taiwan. Therefore, we reviewed current research and the development status of coupled THMC processes in disposal facilities of spent nuclear fuel to investigate the coupled THMC model and propose methods of THMC technical development for HLW disposal in Taiwan. The results from this study furnish THMC-based information and pretechniques for the performance assessment and safety analysis of the final disposal of HLW in Taiwan.

REFERENCES

1. Taipower company, *Final disposal project for spent nuclear fuel in Taiwan*， Taipower company, Taipei (2006).(in Chinese)
2. IAEA, *Geological disposal of radioactive waste: Safety requirements*. Technical Report WS-R-4, International Atomic Energy Agency (IAEA), Vienna (2006).
3. P. Witherspoon, *Geological problems in radioactive waste isolation- second worldwide review,* [LBNL-38915] Lawrence Berkeley National Laboratory, Berkeley, California (1996).
4. P. Witherspoon, *Geological challenges in radioactive waste isolation-third worldwide review*, [LBNL-49767] Lawrence Berkeley National Laboratory, Berkeley, California (2002).
5. P. Witherspoon, *Geological challenges in radioactive waste isolation-fourth worldwide review*, [LBNL-59808] Lawrence Berkeley National Laboratory, Berkeley, California (2006).
6. J. Maßmann, *Modeling of Excavation Induced Coupled Hydraulic-Mechanical Processes in Claystone*, PhD thesis, Institut für Strömungsmechanik, Leibniz Universität Hannover, report no. 77 (2009).
7. W. C. Chen, *The study on swelling behavior of buffer material in a deep geological repository*, Ph.D. Dissertation of Institute of Civil Engineering ,National Central University, Taiwan (2004). (in Chinese)
8. T. Chan, N.W. Scheier and V. Guvanasen, *MOTIF code version 3.2 theory manual. Atomic Energy of Canada Limited for Ontario Hydro*. Ontario Hydro Nuclear Waste Management Division Report No: 06819-REP-01200-0091-R00 (1999).
9. M. Chijimatsu, T. Fujita and A. Kobayashi, *Analyses of Task 2C - DECOVALEX II, progress report*. Japan Nuclear Cycle Development Institute (JNC), Tokai, Japan, and Iwate University, Japan (1999).

10. R. Sato, T. Sasaki, K. Ando, P. A. Smith, J. W. Schneider, *Calculations of the Temperature evolution of a Repository for Spent Fuel in Crystalline and Sedimentary Rocks*. Nagra Technical report 97-02 (1997).
11. J. Rutqvist, J. Noorishad and C. F. Tsang, *Coupled analysis of a thermohydromechanical experiment in rock at Kamaishi Mine*. Report to SKI and DECOVALEX. Lawrence Berkeley National Laboratory, Berkeley, USA (1999).
12. S. M. Tijani, VIPLEF, CHEF, HYDREF - User's Guide. Paris, France: Paris School of Mines (ENSMP) (1991).
13. J. P. Magnaud, S. Goldstein, "The finite element version of TRIO Code", *7 th International Conf. on Finite Element in flow problems*", Huntsville, USA, 1982.
14. P. Verpeaux, A. Millard, T. Charras, A. Combescure, "A modem approach of large computer codes for structural analysis", *Proc. Structural Mechanics In Reactor Technology*, **10**, Los Angeles (1989).
15. M. Board. *UDEC (Universal Distinct Element Code) Version ICG1.5*. Vols. 1-3. NUREG/CR-5429. Washington, D.C.: Nuclear Regulatory Commission (1989).
16. S. H. Luo, Q. H. Qian, J.X. Li, W.B. Zhou, "Deep Geological Disposal of High-Level Nuclear Waste and Its Research Outlines", *Rock and Soil Mechanics*, **26** (Supp.1), 264 (2005). (in Chinese)
17. C. F. Tsang, O. Stephansson, L. Jing, F. Kautsky, "DECOVALEX Project: from 1992 to 2007", *Environ Geol*, **57**, 1221, doi:10.1007/s00254-008-1625-1 (2009).
18. C. F Tsang, "Introductory editorial to the special issue on the DECOVALEX-THMC project", *Environ Geol*, **57**, 1217, doi 10.1007/s00254-008-1626-0 (2009).
19. H. Zhou, X. T. Feng, "Advances in Coupled Mechanical-Hydro-Chemical Processes in Rocks", *Chinese Journal of Rock Mechanics and Engineering*, **25**(4), 855 (2006). (in Chinese)
20. L. Jing, C. F. Tsang, O. Stephansson, "DECOVALEX—an international cooperative research project on mathematical models of coupled THM processes for safety analysis of radioactive waste repositories", *Int J Rock Mech Min Sci*, **32**, 389 (1995).
21. L. Jing, O. Stephansson, C. F. Tsang, F. Kautsky, *DECOVALEX— mathematical models of coupled T-H-M processes for nuclear waste repositories—executive summary of phase I, II and III.* Swedish Nuclear Power Inspectorate SKI technical report 96, Stockholm, p58 (1996).
22. C. F. Tsang, O. Stephansson, F. Kautsky, L. Jing, *Coupled THM processes in geological systems and the DECOVALEX project*. pp. 3–16, In: Stephansson O, Hudson JA, Jing L (eds) Coupled thermo hydro-mechanical-chemical processes in geo-systems: fundamentals, modelling, experiments and applications. Elsevier, Oxford (2004).
23. DECOVALEX, 2016, http://www.decovalex.org/index.html
24. L. Jing, F. Kautsky, O. Stephansson, C. F. Tsang, *DECOVALEX-THMC project, executive summary*, Swedish Nuclear Power Inspectorate, Stockholm (2008).
25. O. Stephansson, L. Jing, C. F. Tsang, "Coupled thermo-hydromechanical processes of fractured media—mathematical and experimental studies", In: *Development in geotechnical engineering*, **79**. Elsevier Science, Amsterdam, 575p (1996).
26. O. Stephansson, "Special issue of International Journal of Rock Mechanics and Mining Sciences & Geomechanics Abstracts", **32**(5), 387 (1995).
27. O. Stephansson, C. F Tsang, F. Kautsky, "Special issue of *International Journal*

of Rock Mechanics and Mining Sciences", **38**(1), 1, (2001).

28. O. Stephansson, J. A. Hudson, L. Jing, *Coupled thermos-hydro-mechanical-chemical processes in geosystems: fundamentals, modelling, experiments and applications*, Elsevier, Oxford (2004).
29. L. Jing, O. Stephansson, "Special issue of *International Journal of Rock Mechanics and Mining Sciences*", **42**(5-6), 591 (2005).
30. W. Xu, X. Tan, S. Yang, *Advances on coupled thermo-hydromechanical-chemical processes in geosystems and engineering*, (Proc. Int. Conf. GeoProc 2006, Nanjing, China). Science Press,Beijing (2007).
31. C. F. Tsang, "Special Issue: THE DECOVALEX-THMC PROJECT (Safety assessment of nuclear waste repositories)", Special issue of *Environmental Geology*, **57**(6), 1217 (2009).
32. Institute of Rock and Soil Mechanics, Chinese Academy of Sciences, http://www.whrsm.cas.cn/gjjl/hzxm/200909/t20090906_2466489.html (2016) (in Chinese)
33. Y. F. CHEN，C. B. ZHOU，X. Y. MAO，L. R. JING, "Numerical simulation of coupled thermal elastic behaviors for hard rock pillar in Äspö Pillar Stability Experiment, Sweden", *Chinese Journal of Geotechnical Engineering*, **23**(8), 1200 (2010). (in Chinese)
34. D. E. Keyes et al., "Multiphysics simulations challenges and opportunities. Int. J. High Perform", *Comput. Appl.* **27**(1), 4 (2013).
35. S. Balay et al., *PETSc Users Manual*. Technical Report. Argonne National Laboratory (2013).
36. S.P. Zwart et al., "A multiphysics and multiscale software environment for modeling astrophysical systems", *New Astron.* **14**(4), 369 (2009).
37. B. Patzak, Z. Bittnar, "Design of object oriented finite element code", *Adv. Eng. Softw.* **32**(10), 759 (2001).
38. D. Trebotich, B. V. Straalen, D. Graves, P. Colella, "Performance of embedded boundary methods for CFD with complex geometry", *J. Phys.: Confer. Ser.*, **125** (1), 012083, (2008). (Available from http://stacks.iop.org/1742-6596/125/i=1/a=012083⟩.
39. A. Logg, K. A. Mardal, G. Wells, *Automated Solution of Differential Equations by the Finite Element Method: The Fenics Book*., Springer-Verlag, Berlin Heidelberg (2012).
40. COMSOL, 2016. *Introduction to Comsol Multiphysics®*: Version 5.2, COMSOL.
41. D. L. Parkhurst, C. A. J. Appelo, *User's guide to PHREEQC (Version 2) — A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations*, U.S. Geological Survey Water – Resources Investigations Report 99-4259, U.S. Geological Survey, Denver, Colorado, 310pp (1999).
42. S. R. Charlton, D. L. Parkhurst, "Modules based on the geochemical model PHREEQC for use in scripting and programming languages", *Comput. Geosci.*, **37** (10), 1653 (2011).
43. USGS, *PhreeqcI--A Graphical User Interface for the Geochemical Computer Program PHREEQC (*2014*).* http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqci/
44. Mathworks, *MATLAB User's Guide*. Inc., Natick, MA, 5 (1998).
45. L. Wissmeier, D. A. Barry, "Simulation tool for variably saturated flow with

comprehensive geochemical reactions in two- and three-dimensional domains", *Environmental Modelling & Software*, **26**, 210 (2011). doi:10.1016/j.envsoft.2010.07.005

46. S. C. Seetharam, D. Jacques, "Developments in a Coupled Thermal-Hydraulic-Chemical Geomechanical Model for Soil and Concrete", *2013 COMSOL Conference*, Rotterdam (2013).
47. O. Nasir, M. Fall, E. Evgin, "A simulator for modeling of porosity and permeability changes in nearfield sedimentary host rocks for nuclear waste under climate change influences", *Tunnel. Undergr. Space Technol.* **42**, 122 (2014).
48. A. Nardi, A. Idiart, P. Trinchero, L. M. de Vries, J. Molinero, "Interface COMSOL-PHREEQC(iCP), an efficient numerical frame work for the solution of coupled multiphysics and geochemistry", *Comput. Geosci*. **69**, 10 (2014).
49. D. Jacques, J. Šimůnek, *User manual of the multicomponent variably-saturated flow and transport model HP1: description, verification, and examples. Version 1.0*, BLG-998. Waste and Disposal, SCK.CEN (2005).
50. K. U. Mayer, *MIN3P V1.0 User Guide*, University of Waterloo, Department of Earth Sciences, 26.06.00 (2000).
51. C. Zheng, P. Wang, *MT3DMS Documentation and User's Guide*, (1998).
52. J. Rutqvist, C. F. Tsang, "TOUGH-FLAC: a numerical simulator for analysis of coupled thermal-hydrologic-mechanical processes in fractured and porous geological media under multi-phase flow conditions", In: *Proceedings of the TOUGH Symposium 2003*, Lawrence Berkeley National Laboratory, Berkeley, May 12–14, 2003 (2003).
53. T. Xu, E. Sonnenthal, N. Spycher et al., "TOUGHREACT—a simulation program for non-isothermal multiphase reactive geochemical transport in variably saturated geologic media: applications to geothermal injectivity and CO2 geological sequestration", *Comput. Geosci.*, **32**, 145 (2006).
54. H. P. Cheng, G. T. Yeh, "Development and demonstrative application of a 3-D numerical model of subsurface flow, heat transfer, and reactive chemical transport: 3DHYDROGEOCHEM", *J. Contam. Hydrol.*, **34**(1–2), 47 (1998).
55. J. Taron, D. Elsworth, K. B. Min, "Numerical simulation of thermal-hydrologic-mechanical-chemical processes in deformable, fractured porous media", *Int. J. Rock Mech. Min. Sci.* **46**(5), 842 (2009).
56. Q. Li, K. Ito, Z. Wu, C.S. Lowry, and S.P. Loheide II, "COMSOL multiphysics: A novel approach to ground water modeling". *Ground Water* **47**, 480 (2009).

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