Task Specifications for DECOVALEX-2023

Supplemental information for DECOVALEX-2023 agreements

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Introduction

This document provides short summaries of the tasks accepted for the next phase of DECOVALEX-2023. All the proposals presented here are subject to change as the tasks develop, but any changes will be in full discussion with the funding organisations and research teams.

Table 1 gives a summary of the tasks being proposed with links to the appropriate section. Tasks are ordered alphabetically by the organisation of the proposer.

Task Summaries

A standard template has been used for the proposals to give an overview of the suggested tasks. Proposers were asked to use approximately two pages for their task suggestions – this has not been adhered to in some cases.

Task letters have been updated to be consistent with the DECOVALEX-2023 contracts and financial information.

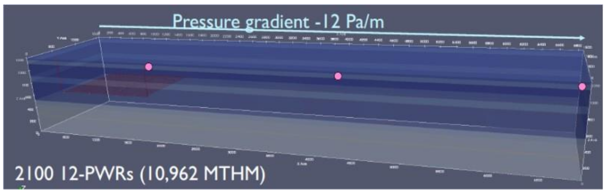
Table 1. Summary of the tasks. The task number in the table is linked to the section giving the summary (ctrl+click to follow the link).

ID	Short Name[1]	Title	Organisation	Processes	Primary Material Type	Task Lead
A	HGFrac	Heat and Gas Fracking	Andra	THM + gas	Argillite	Xxxxx xxxx
B	MAGIC	Modelling Advection of Gas In Clays	BGS	HM + gas	Engineered Clay	Xxx xxxxxxxxxx
C	-	Modelling THM processes at the Full-Scale Emplacement (FE) heater experiment	ENSI/Quintessa	THM	Argillite	Xxxxxx xxxxxxxx xxxx xxxxxxx
D	-	Full-scale Engineered Barrier System Experiment at Horonobe URL	JAEA	THM(C)	Sedimentary	Xxxxxx xxxxxxx
E	BATS	Heated Brine Availability Test in Salt	Sandia NL	THMC	Evaporitic Salt	Xxxxxxxx xxxxxxxxx
F	-	Proposed PA/UQ/SA Benchmarking Task	Sandia NL	PA – THMC	Crystalline focus and possibly salt	Xxxxx xxxxxx
G	SAFENET	Safety Implications of Fluid Flow, Shear, Thermal and Reaction Processes within Crystalline Rock Fracture Networks	UFZ	THMC	Crystalline focus plus greywacke	Xxxx xxxxxxx, xxxxx xxxxxxxx, Xxxxx xxxx xxxxxx

[1] Summaries were not required to have a short name

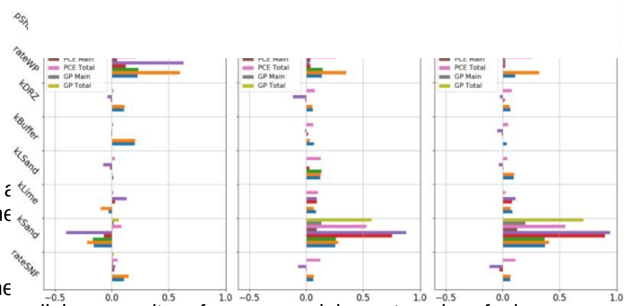
Task F: Proposed PA/UQ/SA Benchmarking Task;

Outline Description



Proponent: Department of Energy, DOE, USA

Objectives of the task: This task is intended to build confidence in the models, methods, and software used for performance assessment (PA), or safety assessment, of deep geologic repositories, and/or to bring to the fore additional research and development needed to improve PA methodologies. The objectives will be accomplished through a staged comparison of models and methods used in different PA frameworks, including: (1) coupled-process submodels (e.g. waste package corrosion, spent fuel dissolution, radionuclide transport, etc.) comprising the full PA model; (2) deterministic simulation(s) of the entire PA model for defined reference scenario(s); (3) probabilistic simulations of the entire PA model; a analysis (SA) methods/results for probabilistic simulations of define



Rock types and engineered materials to be considered: On the U.S. DOE proposes working with two generic reference cases in parallel: a repository for commercial spent nuclear fuel (SNF) in a fractured crystalline host rock and a repository for commercial SNF in a bedded salt formation. Over the past several years, the U.S. disposal program has developed a suite of reference cases to conduct 3D probabilistic performance simulations of generic repositories in a variety of host rocks. The DOE crystalline and salt reference cases could be used as valuable starting points to define DECOVALEX test cases. Specific features and characteristics of the natural and engineered systems for inclusion in the generic DECOVALEX test cases will be determined by the task group in order to create problems that are of interest to all participants. Although a direct comparison cannot be made between simulations of a crystalline repository and simulations of a salt repository, it is expected that lessons learned regarding, for instance, methods of coupling process models, propagating uncertainty, or conducting sensitivity analysis will be transferable between concepts.

Principal experimental data: Thermal, hydrological, mechanical, and chemical properties of individual components of the engineered and natural systems, constitutive relationships, and other characteristics such as fracture network distributions will be chosen for relevance to participating task members. DOE proposes characterizing the reference case systems using data and measurements collected at relevant underground research laboratories (URLs), field sites, and from past DECOVALEX-related laboratory experiments, such as those exploring coupled processes in compacted bentonite.

Data scale and duration: Available URL tests and data are necessarily of very short duration compared to a repository performance assessment but may be of value in helping to “validate” the implementations of coupled process models incorporated into PA frameworks.

Relevance to radioactive waste disposal safety cases (Performance and Safety Assessment):

This task is a Performance and Safety Assessment task.

Applicability to other disposal concepts/rock types/engineered materials: This task will compare a range of performance assessment approaches and as such will produce a set of best practices and will allow for mutual learning among participants. These best practices, while developed with a focus on one or perhaps two rock types, will be transferrable to other PAs for other rock types.

Special and/or novel features: This task is different from typical DECOVALEX modelling tasks in that it does not focus on a particular set of experiments. Comparing PA/UQ/SA approaches and practices is a novel task for the DECOVALEX family.

Relevance to non-radioactive waste management applications: Some relevance to other geologic and complex system problems that have highly coupled processes, large data sets and significant uncertainties, such as resource extraction and remediation processes, including fossil fuel and minerals.

Summary of Proposed Work

Description and Justification of the Technical Focus

Performance assessment (PA) is a "quantification of the overall level of system performance, analysis of the associated uncertainties, and comparison to the relevant design and safety standards." Quantitative PAs are an important contribution to the development of the long-term safety case for deep geologic disposal of radioactive wastes. Yet there are many differences among national programs as to how PAs are conducted, for example in the way different sources of uncertainty are accounted for, including scenario uncertainty, conceptual model uncertainty, and parameter uncertainty. Some programs choose to propagate the full ranges of these uncertainties through the PA model, resulting in a probabilistic distribution in the performance or safety metric. Other programs conduct a "deterministic" PA using representative or "best estimate" values for input parameters and models, as well as stylized or conditional scenarios, e.g., the assumption that a human intrusion event occurs at a specific future time and damages a specified number of waste containers. Other programs use a combination of probabilistic and deterministic calculations.

Other differences among national programs may stem from the approach for incorporating individual component models into the total system model. In particular, heat-generating waste generally results in strong and often non-linear coupling between multiple thermal-hydrologic- chemical-mechanical (THCM) processes, which can be numerically challenging to represent and solve in a large-scale, high-dimensionality system model with parameter uncertainties. The trend in recent years has been to lessen the use of decoupled submodels and other simplifications in a system level model. This has been made possible by advances in computer power, which allows the use of higher spatial dimensionality, more realistic and detailed spatial heterogeneity, and direct numerical solutions of coupled THCM processes in one detailed system model rather than a sequence of loosely connected submodels (connected only via mass transport). However, some simplifications and reduced-order or surrogate models (reduced in dimensionality, coupling, scale, and data) are still necessary for the foreseeable future, especially for multi-realization, probabilistic PAs. The task proposed by DOE will compare and contrast the different approaches to conducting PAs by different national programs with an eye towards building confidence in the safety case. By using the same generic reference case repository, the comparison will be more direct among the different national programs and it is hoped that a set of best "system modelling" practices can emerge from this collaborative effort.

Proposed Work Programme

An incremental approach to the development of this task is proposed based on the logical workflow of a system performance assessment:

- **Step 1: Definition of Reference Cases/Scenarios.** Completely describe the features, events, and processes (FEPs) to be simulated in each reference case (crystalline and salt). Each reference case will define (1) fuel type, burn-up, and inventory (and associated heat output), as well as the instant release fraction and probably an agreed-up dissolution mechanism; (2) buffer material and properties, such as bulk density, porosity, permeability, and thermal conductivity; (3) waste package material, thickness, dimensions, and corrosion/failure mechanism(s); (4) natural system properties, including regional gradient/boundary conditions and stochastic parameters for discrete fracture networks (DFNs); and (5) performance scenarios to be considered, such as a natural evolution and/or glacial disruption scenarios for the crystalline case and a human intrusion scenario for the bedded salt case. The group will agree upon a defined output metric(s) that can be used for comparisons of the PA frameworks, such as aqueous-phase concentration of one or more agreed-upon radionuclides at defined locations in the model domain. The initial description will be for a deterministic case; prior to UQ/SA a full description of uncertain parameters and their distributions will be necessary.
- **Step 2: Comparison of subsystem models.** Comparison of PA software and process model implementations on a variety of subsystem process models (or groups of submodels), such as waste package failure rate/degree; near-field radionuclide source term (e.g., radionuclide mass flux exiting the buffer); heat conduction and convection; bulk fluid phase movement; etc. will ensure a common understanding of problem definitions and verify/validate model and software implementations against each other.
- **Step 3: Comparison of a full deterministic PA model.** Compare simulations of the full system PA model using the chosen metric(s).
- **Step 4 (optional): Quantification and propagation of parameter uncertainty**. The task group may investigate a variety of UQ methods commonly employed in safety assessments, such as fitting continuous distributions (data-rich parameters/models) and subjective probability distributions (data-poor models that require expert elicitation or other methods). Regardless, the group should address suitable methods of propagating uncertainty from one submodel to another.
- **Step 5: Uncertainty analysis and comparison of full probabilistic PA models and major submodels.** Evaluate the impact of various types of uncertainties, including parameter uncertainty, stochastic field uncertainty (DFNs), and conceptual model uncertainty. This will be quantified by comparisons of the uncertainty distributions of agreed-upon output parameters and their associated statistics, such as mean and median. Of special interest is the effect of using alternative conceptual and/or constitutive models for buffer behavior, host rock performance, etc. on both near-field performance (e.g., radionuclide flux to the host rock) and total system performance. A noteworthy question in this context is the use of high-fidelity process models vs. simplified representations or surrogate models, in particular for complex coupling between processes and/or strongly non-linear processes (e.g., thermally-induced coupled processes, non-linear chemistry, etc.). Given its focus on a deep fundamental understanding and analysis of coupled processes, the DECOVALEX group is in a unique position to answer such question.
- **Step 6: Sensitivity Analysis.** For comparisons of probabilistic PA results, the group will conduct sensitivity analyses (SA) using an agreed-upon suite of SA methods and metrics,

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including more traditional methods such as correlation coefficients and linear regression and less common methods (in past safety assessments) such as variance-based methods. Each country may use the PA results from their own model or, perhaps more likely, the task group may decide to choose one set of PA model results for comparison of SA methods and results.

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U.S. DEPARTMENT OF ENERGY

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