



**Appendix A:
Specification
For
UKRI-2370
Expert Numerical Support in the
Analysis of Thermo-Hydro-
Mechanical-Gas (THMG) Datasets**



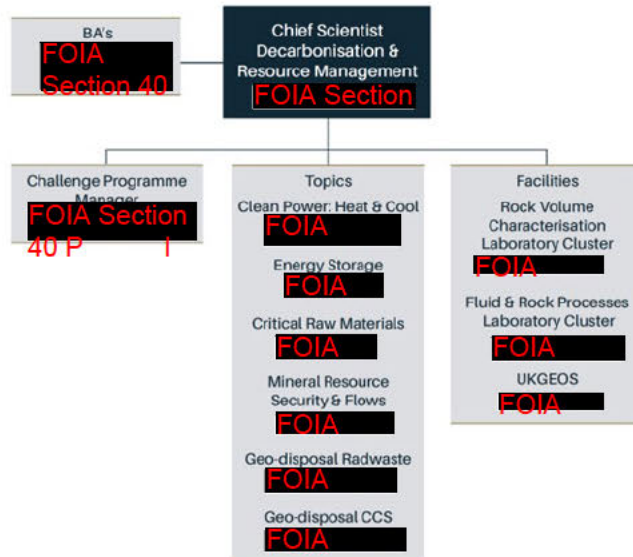
1 Introduction

To build on existing expertise and relationships developed since 2021, the Radioactive Waste team at the British Geological Survey are seeking numerical modelling expertise to input to a number of our on-going commissioned research projects. These projects, within the Radioactive Waste Disposal Research Team, are centred on enhancing understanding on the multi-phase (gas, fluids) flow within, and deformation of, low permeability materials being considered as a host-rock and for the engineering components of a deep repository for higher activity radioactive waste internationally. These projects include but are not limited to DECOVALEX 2023, EURAD GAS and EURAD Hi-TEC.

The Specification builds on previous work and is to continue the analysis/interpretation of large datasets linked to multiphase flow and deformation testing, peer review exercises and publication and presentation of outputs.

2 Background to the Requirement

The successful Supplier will report directly to **FOIA Section 40 Personal** within the Radwaste Team and Fluid and Rock processes Laboratory Cluster, part of Decarbonisation and resource management (see organogram below).



Both Teams have an extensive track record of science excellence spanning the last 30+ years, and the successful Supplier will need to demonstrate a detailed knowledge of the Teams' research and outputs.

The Teams work closely with regulators and implementors on a range of topics, from the disposal of radioactive waste to gas storage (information on specific activities can be found on the BGS website, <https://www.bgs.ac.uk/>). It is important the successful Supplier has a proven track record of successful collaboration and engagement in the delivery of science relating to low permeability materials.

The successful Supplier will be responsible for the provision of expert numerical input into a host of projects (see Sections 3 and 4 below) relating to multi-phase flow and mechanical analyses. They will also be required to help in the derivation of flow and constitutive laws e.g. the description of time dependent deformation processes. They must have expert knowledge of coupled THMG processes and their implementation in numerical modelling codes. An important part of the role, will also be to support BGS colleagues in the development of their science, through but not limited to, the development of algorithms in the processing and manipulation of time series data.

3 Scope

The scope of work includes undertaking a wide variety of tasks associated with the delivery of the projects' objectives set out in Section 4 below.

The tasks to be undertaken will be discussed and agreed between BGS and the Supplier following appointment and will amount to a maximum of 10 person days per month for a period of 36 months (plus possible extension of a further 12 months) or, to a maximum budget limit of £100,000. These tasks may involve, but are not limited to:

- Development of mathematical and numerical models to advance the understanding of coupled thermo-hydro-mechanical processes in low permeability geological systems.
- Numerical support and interpretation of bespoke laboratory and field-scale experimentally derived thermo-hydro-mechanical datasets including numerical representation of consolidation, hydraulic permeability and two-phase flow behaviours
- The development of bespoke finite element codes tailored for (i) Single-phase (gas/water) flow simulations (ii) Mechanical deformation processes (iii) Fracture development (iv) The application of stochastic approaches to the characterization of geological systems
- Responding to general numerical enquiries (within 48 hours, unless otherwise agreed) relating to BGS research.
- Expert contribution to project outputs including BGS and client reports, associated papers and oral contributions.
- Critical analysis of models and codes prepared by participants of the Decovalex D-2-23 Task B project.
- Workshop participation including international travel to attend Decovalex, EURAD and other project meetings.
- It is anticipated work tasks will be undertaken remotely, however, there may be a requirement to travel to the BGS head office (Keyworth) to attend meetings or to international DECOVALEX and EURAD meetings. All reasonable expenses, in line with standard BGS procedures and protocols, associated with such travel will be met by BGS.

It is anticipated services (i.e. number of days worked per month) supplied by the Supplier may increase or decrease depending on BGS requirements. Any changes to the initial scope of up to 10 days/month will be agreed between BGS and the Supplier in advance.

Suppliers should note that the 10 days/month is not guaranteed.

The Supplier's day rates are calculated on the basis of an eight-hour day.

4 Requirement

The Supplier shall carry out the agreed works, in accordance with the following process:

- i. BGS will issue a single purchase order covering “Numerical Support to Radioactive Waste Disposal Research’.
- ii. Following acceptance of the purchase order, the Supplier will work with BGS to define the detailed scope of works, deliverables and timescales. The detailed programme of work may evolve to reflect the development of the research project. The Supplier and BGS will agree any changes to the programme of work collaboratively. The programme of work will amount to (a maximum of) 10 person days of work per month for a period of 36 months (and a possible extension period of 12 months).
- iii. The Supplier will carry out the task in a prompt and timely manner. One invoice will be submitted monthly by the Supplier covering progress against all tasks carried out since the previous invoice. Each task shall be itemised individually on the invoice, using the agreed name and reference number.
- iv. Weekly meetings, unless otherwise specified, will be held at which the Supplier to present progress and agree subsequent work for the following week.
- v. The Supplier will be expected to reply to requests for work by BGS within two working days or less of notification and if necessary adjust activities to reflect the changing requirements of BGS.

Suppliers should note that some projects may require the Supplier to possess Cyber Essentials certification and to basic level BPSS clearance. Therefore, it is a desirable requirement of the Contract for the Supplier to hold such credentials.

Specific activities and expectations are covered below:

Aims and objectives of BGS components of the Decovalex, EURAD GAS and Hi-tec, Andra-BGS gas and water flow in CO_x, BGS National Capability projects which form the core of activity within this requisition

Task 1: Decovalex 2023

The DECOVALEX project is an international research and model comparison collaboration, initiated in 1992, for advancing the understanding and modelling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems. BGS manage Task B of the current phase (Decovalex2023) focussed on the advective modelling of gas flow in clay (<https://decovalex.org/>). The objective of this task is for participating organisations (teams) to develop models to better represent the complex processes controlling advective gas flow.

Activity 1: Conceptual model development phase. The main objective of this first stage is to assess teams' modelling capabilities. Participating teams will focus on how their models describe the development of dilatant pathways, the permeability associated to this pathway development and the coupling between permeability and stress. A one-dimensional gas test data modelled in an earlier Decovalex phase (D-19) will be made available for those participants who did not take part in the previous Decovalex phase. Optionally, teams will be able to test their models against this dataset and, if needed, improve their numerical procedures. BGS are tasked with assessing models and results presented at project meeting.

Activity 2: Blind prediction test. The main objective of this stage is to assess models from Activity 1 and to analyse each team's capabilities against a new dataset. Special emphasis will be placed on the fact that the purpose of this test is not to calibrate the models via fitting routines but to analyse whether the key features of the experiments are well-captured or not. BGS will assess the performance of the codes and present assessments at progress meetings.

Activity 3: A full-scale in situ test. In this activity, teams will be required to model a large-scale gas injection test (Lasgit) experiment conducted at the Äspö Hard Rock Laboratory. BGS will critical analyse the models and present assessments at progress meetings.

Activity 4: Workshop participation. BGS will lead a series of workshops in various places internationally to present analysis of participants modelling, provide support and communicate with the participants. Activity 5: final report and paper publication. A final report will be led by BGS critically analysing Activities 1 through 4, appraising the models, assessing their function and performance for both inverse and predictive modelling, and help to define a series of recommendations regarding future model development.

Task 2: EURAD gas and Hitec

This is a five year programme of work (starting 2019), part funded by the EC, RWM, COVRA and ONDRANIRAS, in which BGS has been commissioned to perform laboratory diagnostic tests examining the processes governing the diffusion and advection of gas through a range of clay-based materials.

Gas: Activity is split into a number of work packages focussed on the diffusion and advection behaviour of gas in engineered barriers, synthetic materials and clay host rocks. Experiments are performed under triaxial, isotropic and constant volume boundary conditions. The role of fractures and fracture self-sealing is also explored using shear box experiments, supported by fracture visualisation tests (e.g. <https://pubs.geoscienceworld.org/minmag/article/79/6/1335/300906/The-visualization-of-flow-paths-in-experimental>). The experimentally derived data will be appraised including inverse modelling of gas and hydraulic data to define experimental constants, mechanical modelling to support interpretation of stress field monitoring, development of algorithms to support analysis of large datasets.

Hi-tec: As above, with activity split into work packages examining the influence of heat on the development and evolution of swelling pressure, porewater pressure, permeability and mechanical behaviour. Single-phase models will be developed to examine permeability and pore pressure development during thermal cycling as well as inform on different theoretical approaches to the modelling of thermo-hydro-mechanical behaviour.

Task 3: Gas and water flow in CO_x

Working closely in collaboration with Andra, BGS has an experimental programme of work examining the gas and water flow behaviour of CO_x. As part of your role, you will be responsible for analysis of transient and steady state data to derive THMG properties and help colleagues to provide critical insight into the fundamental controls governing advection, diffusion and the mechanical behaviour of CO_x.

Task 4: National Capability

As part of its national capability role, BGS has a programme of research linked to flow and deformation within the geosphere to further understanding of the impact of sub-surface activities such as waste disposal and energy storage. As part of this role, BGS undertake experiments and field measurements to define hydraulic, gas and mechanical behaviour of materials including clay-based barriers, clay formations, halite and general porous media (e.g. sandstones). These experiments will require numerical modelling of current and future data to define the consolidation, hydraulic and gas properties of different subsurface materials. Work will primarily focus on low permeability material such as the CallovoOxfordian claystone, Opalinus Clay, Boom Clay, halite and cementitious and clay-based engineered materials.

5 Timetable

This Contract will take effect from 1st February 2023 and is anticipated to run until January 31st 2026. The Contract may be extended for a period of 12 months provided the Supplier is given 3-months notice. The Supplier will raise monthly invoices to cover work performed in arrears against agreed activities specified in the weekly meetings with Dr Jon Harrington. This will facilitate metrics to be easily assessed and allow prompt payment from BGS to the Supplier.

Specific activities will include, but are not limited to:

- participation in DECOVALEX 2023 Spring 2023 (South Korea) including preparation and presentation of Task B activities
- participation in DECOVALEX 2023 Fall meeting (France) including preparation and presentation of Task B activities
- completion of DECOVALEX final report (September 2023) including synthesis of activity within Task B
- completion of DECOVALEX final peer review paper for Task B focussed on modelling results from the Lasgit experiment (December 2023)
- participation in EURAD meeting throughout 2023-2024 (various locations, some face-to-face) including analysis and presentation of data and supportive numerical modelling
- help in the preparation of interim reports for Andra December 2023, 2024 and 2025
- help in the completion of EURAD reporting throughout 2023 and up to July 2024
- contribute to future projects which arise during the period covered by the contract
- peer review work for national capability and external income projects
- Support in the preparation of proposals