# ANDRA THESES
# 2021 CALLS FOR PROPOSALS
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# TOPICS

*Introduction*

*R&D work is carried out throughout the life of radioactive waste repositories, from design through operation and closure, as needs arise. The gradual nature of the development of disposal facilities over several decades, or even a century for the Industrial Centre for Geological Disposal (Cigeo), means that they can be optimised continuously with the integration of advances in knowledge.*

*To conduct its research work, Andra has relied on the expertise of the national and international R&D and innovation network for more than 25 years. Andra also supports training through research through a call for thesis projects. For several years, Andra has also had its own research tools: (i) the Underground Research Laboratory and the Perennial Observatory of the Environment, in Meuse/Haute-Marne, specifically for the Cigeo project, and (ii) digital simulation resources for all of Andra's activities.*

*This new 2021 Andra call for thesis projects is taking place in this context. It aims at covering a range of diverse topics with short- and medium-term operational challenges. These topics mainly concern the Cigeo project, but some are also relevant for surface centres.*

*Essentially, it's a question of tackling complex issues, in particular multiple couplings in the broadest sense, in order to better quantify the design and safety margins in relation to the choices made and to prepare the way for future optimisation in design. The proposed topics aim in particular to get as close as possible to actual repository operation.*

*The associated scientific issues and/or obstacles are significant. The proposed topics thus call for solid scientific and technological knowledge and multiple qualities including a strong aptitude for multidisciplinarity, analysis and cognitive ability, combining experimentation, modelling and numerical simulation. They provide a forum for the expression of the scientific excellence of the laboratories and candidates.*

## Geology – hydrogeology – solute transfer in the natural environment

### 1. Conceptual representation, modelling and numerical simulation of flows and solute transport in the Barrois Limestone Hydrosystem around the Cigeo project

The Industrial Centre for Geological Disposal (Cigeo) for high-level and intermediate-level long-lived radwaste in a deep clay formation in Meuse/Haute-Marne departments includes surface installations that will be located, if the project is accepted, in the Barrois limestone formation. This formation consists of alternating levels of more or less karstified marl-limestone affected by surface weathering (epikarst). Design studies for surface facilities currently take into account the specific hydrogeological characteristics of this formation, following a classical hydrogeological approach of the equivalent continuous porous medium type, considered as bounding.

The thesis research will focus on the development of a model for the explicit representation of flows within the Barrois limestone formation, specifically in and around the ramp zone. On the basis of the developments already carried out, and by applying a global methodological approach to the geological, hydro-geophysical and hydro-chemical characterisation data of the Barrois limestone hydrosystem, it will be a question of developing a conceptual scheme of explicit 3D hydrogeological and hydrodynamic representation, covering scales ranging from the piezometer

to that of a study sector of several square kilometres, and then developing a model relating to one of the spatial scales considered (several hundred metres to several kilometres). The work will be based in particular on the existing measurement network (about 30 instrumented boreholes, 6 hydrological stations, meteorological stations, etc.) installed in recent years.

# Thermo-hydro-mechanical behaviour of the Callovo-Oxfordian formation

## 2. Modelling and numerical simulation of the formation and hydromechanical behaviour of damage at the periphery of tunnel intersections

The damaged (e.g. fractured) zone created in the immediate vicinity of the underground structures in the Callovo-Oxfordian during excavation and its hydromechanical behaviour have been the subject of numerous characterisation and modelling efforts from the scale of the sample to the structure. There is now a solid base of knowledge about this damaged area, including its major role in the hydromechanical behaviour of structures over time. In particular, it concerns the linear of the structures. In addition, Cigeo's underground facility will include numerous intersections of structures. At this stage, their design and dimensioning have been carried out conservatively using a bounding approach, particularly in terms of modelling the local damaged area.

The thesis research will focus on the modelling and numerical simulation in 3D of the hydromechanical behaviour of the intersections of structures in the Callovo-Oxfordian, through the explicit representation of the damage induced by the first structure and then by the second structure dug perpendicularly. Approaches such as equivalent continuous porous or discrete (e.g. fractured) medium may be used in the representation, with appropriate justification. The types of planned linings/supports and the methods of excavation and installation, currently selected or possible at this stage of Cigeo's design, are to be taken into account, particularly with regard to comparing the behaviour of intersections.

## 3. Characterisation and micro/macro modelling of the hydromechanical-gas behaviour of clay materials for Cigeo project closure structures

Simulations of the hydromechanical-gas behaviour of closure structures are based on complex models to represent the evolution of the various materials that make up the structures. In particular, models such as the Barcelona Basic Model (BBM) and its extension Barcelona Expansive Model (BExM), which introduce two levels of structure associated with micro- and macropores, are used to model the evolution of resaturation, particularly under gas transfer stress of these clay materials in relation to their shaping (pellets, etc.). These models require good knowledge of the hydromechanical-gas interactions between the micro- and macrostructure, in particular under gas transfer stress, and the definition of the representative elementary volume (REV) with its gas hydromechanical characteristics for detailed modelling of the closure structure component of multi-metric to multi-decametric dimensions. The combined use of X-ray and neutron tomography at different sample sizes may make it possible to analyse both the deformation fields and the evolution of water distribution in clay materials during saturation under gas stress.

The thesis research will focus on (i) the development of a technique for the analysis of water transfer and deformation fields under gas stress, (ii) the acquisition of relevant parameters (e.g. interaction functions) for BExM-type models at relevant spatial scales, (iii) the development of hydromechanical-gas evolution models of clay materials at relevant scales, in particular for an actual structure.

# Radionuclides – Radioactive waste

## 4. Speciation and stability of selenium redox states at the interface between Callovo-Oxfordian and HLW disposal cell

Selenium (Se) can have different oxidation states (-II, -I, 0, +IV, and +VI). The -II, -I and 0 states are commonly predominant in "reducing" anoxic environments, while the +IV and +VI states predominate in "oxidizing" environments. In the reducing geochemical environment of the Callovo-Oxfordian (deep clay formation selected for the location of the deep geological repository Cigeo), selenium is thus expected to be thermodynamically stable in solution in redox states ranging from 0 to -II. The solubility of selenium depends on the oxidation state: (a) Se(+VI) and Se(+IV) highly soluble (solubility not controlled by a mineral phase); (b) Se(0), extremely poorly soluble native selenium; and (c) Se(-I) and Se(-II): poorly soluble but significantly more soluble than Se(0). The transition from one oxidation state to another may therefore be accompanied by changes in solubility. However, selenium can remain "metastable" under a high oxidation state +VI far from thermodynamic equilibrium (e.g. redox-reducing domain), especially in the absence of microbial catalysis and specific solids such as certain iron-bearing phases, and be present under different oxidation states in Callovo-Oxfordian pore waters.

The thesis research will focus on the metastability or non-metastability of selenium (VI) and its coexistence with a reduced redox state (-II) under the conditions of the Cigeo project and, namely, between a disposal cell, in this case vitrified high-level waste (HLW) cell containing steel components, corrosion products and the Callovo-Oxfordian. The research shall include day laboratory tests (solubility, speciation, sorption-reduction, etc.) and reactive transport modelling at the scale of a cell, in order to obtain a representation that is as detailed and as reasonable as possible of the multi-scale and multi-component geochemical system (HLW cell and Callovo-Oxfordian).

# Multiple couplings: Disposal materials and components

## 5. Modelling and numerical simulation of the hydromechanical behaviour of the Cigeo project's clay-based closure structures, coupled with hydraulics (resaturation/saturation) and an alkaline disturbance

The Cigeo project's underground facility will be closed and sealed after completion of operations. The galleries will be backfilled with excavated Callovo-Oxfordian clays and swelling clay seals will be placed in the galleries at specific locations and in the access works (shaft and ramp zone). The evolution of the seals and the backfilled galleries after closure will be characterised by a resaturation coupled with an alkaline disturbance that will persist after reaching complete saturation. The design and dimensioning of these closure structures takes these processes into account, in particular in a conservative bounding approach based on simplified numerical simulations and modelling.

The thesis research will focus on the modelling and "fully coupled" simulation in 2D/3D of the hydromechanical behaviour of closure structures with an explicit representation of the coupling with the alkaline disturbance. Using current knowledge on alkaline disturbance in clay environments and the hydromechanical behaviour of materials based on clay rock and swelling clay, in terms of processes, representation models and numerical simulation codes, the thesis will focus on establishing a conceptual scheme of the complete coupling, defining one or more coupling models and conducting numerical simulations (coupling of existing codes in hydromechanics and reactive transport or "fully integrated" coupling in the same code).

# Observation-surveillance: technical devices

### 6. Development of an innovative system for continuous pH measurement in a local or distributed manner (clay, cement or open media)

The pH is a parameter/indicator of many processes for the durability of the structural components of a repository and the behaviour of the surrounding environment (geological environment, open environment). A variety of pH measuring devices already exist today, with limitations including the need for regular, manual calibration, sometimes prior to each measurement.

The thesis research will focus on the development of innovative techniques or methods, for example all-solid-state electrodes, where all the reference electrodes are made from durable materials. Special attention shall be given to the miniaturization of the sensor in order for minimal intrusion. For example, research may include the development and characterisation of perovskite oxides for pH sensors or the use of fibre optic technologies as a pH optode.

# Numerical simulation, BIM, AI for data processing

### 7. Local sensitivity analysis applied to the numerical simulation of strongly coupled physical and/or chemical problems

The post-closure water and gas flow assessment of the Cigeo project is the subject of multi-parametric multi-scale sensitivity studies (from disposal cells to the overall repository with the surrounding geological environment) using probabilistic tools. In particular, they take into account the variabilities and uncertainties of the parameters of gas generation and water and gas flow models. They lead to the definition of sensitivity ranges for flow indicators and thus make it possible to rank the level of uncertainties on the parameters. This approach is comprehensive and has accuracy limits for small parameter value set ranges.

The thesis research will focus on the analysis, selection and development of local intrusive-type sensitivity, in particular automatic differentiation methods (adjoint state-type) for the numerical simulation of water and gas flow in porous media, for localised ranking of the level of influential parameters using deterministic data sets.

# Environment

### 8. Study of landscape structures for the maintenance and optimisation of associated ecosystem services

For the design of the Cigeo project in Meuse/Haute-Marne, Andra set itself the requirement to minimise the project's impact, using the avoid, reduce and offset method. This includes impacts on the ecosystem services provided by the project's host location, in particular with the goal of preserving and enhancing existing landscape structures or creating new ones. Indeed, landscape structures (hedges, copses, ditches) are essential elements for the proper functioning of ecosystems by providing shelter, food and nesting areas for many species. In addition, they are natural barriers to the elements (wind and rain), thus protecting agricultural and livestock activities. Finally, they also correspond to the green grid that provides continuity between ecosystems. The application of this requirement is reflected in the impact study included in the application for the declaration of public utility for the Cigeo project filed by Andra in August 2020.

The thesis research will focus on the functional optimisation of landscape structures from a methodological point of view, taking into account the specific biophysical, biodiversity and land use characteristics of the host location of the Cigeo project so as to further promote the maintenance over time of the ecosystem services, for example pollination services, reduction of

bio-aggressors, maintenance of biodiversity, etc. The impact on ecosystem services of these structures and their design can be assessed by studying existing analogues and/or simulations in the context of environmental modelling at the local scale. Within this framework, in situ experimentation may also be proposed.