

Timodaz School

First Training Course

THM behaviour of clays in deep excavation with application to underground radioactive waste disposal

July 7th – 9th, Lausanne

Simulation with LAGAMINE of a simple THM coupled case. Scoping calculations

Numerical Modeling Exercise

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1. INTRODUCTION

In the continuation of the exercise on laboratory experiment, this exercise session aims to model a simple case of thermo-hydro-mechanical processes in a host formation around a gallery of nuclear waste disposal. This simulation will be performed with the LAGAMINE finite element code. The excavation phase, the drainage of the gallery and the heating phase due to the heat-emitting waste will be modelled.

In the analysis of results, the main thermo-hydro-mechanical processes will be underlined. In particular, the convergence of gallery wall due to excavation, the effect of pore water pressure dissipation upon the drainage of the gallery and the effect of heating in terms of pore water pressure, displacement and effective stress evolutions around the gallery will be discussed.

Within the scoping calculations of the TIMODAZ project, some specific host formations were not considered, but we tried to evaluate the behaviors of a range of argillaceous formations, from plastic (PC) to indurated (I1, I2) clays, as representative of the main underground laboratories in clayey layers. Due to lack of time, the aim of this exercise session is to focus on the plastic clay.

The objective of these calculations is thus to study, numerically, the THM responses of the host formations under different conditions and thus to have an insight on the most critical conditions (important influencing factors) for the THM behavior of the host formation including the thermal limits of it.

2 MODELISATION OF THE CLAY REPOSITORY

2.1 GEOMETRY

We propose to treat the problem as a two-dimensional problem (Plane strain) that is an idealization of the excavation of a cylindrical cavity in a porous isotropic infinite medium (with anisotropic stress state). The excavation will eventually be followed by a liner installation of thickness "e" which allows a given convergence α^{exc} and a heating phase corresponding to the injection of a given thermal flux at the lining. Let's note that gravity is not considered in this modeling.

The segment AB represents the tunnel wall. The inner radius R_0 is equal to 2 m for PC clay. The external radius R^{ext} of the problem is chosen at least 100 times the tunnel radius to be sure that the stresses on the external boundary are not influenced, thus we chose $R^{ext} = 200$ m.

An interface element is placed between the liner and the gallery wall. It allows the passage of heat flux and water flow once the two elements are in contact.

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Figure 1: Problem geometry

2.2 CONSTITUTIVE MODEL AND PARAMETERS

We propose to use the constitutive parameters determined during the first exercise session. Two mechanical constitutive models will be considered during this exercise: a Mohr-Coulomb model (elasto-perfect plasticity) and an Original CamClay model (ACMEG). A thermo-hydraulic coupled law will be also used to tackle the flow problem and the thermal one, as well as the coupling effects. In this model, the variation of temperature induces only elastic deformations.

Here are the thermo-hydro-mechanical characteristics of the plastic clay constituting the repository (Table 1 and 2). The properties are given for the initial temperature and pore water pressure. However, we suppose that the parameters are temperature independent.

Hydraulic characteristics		PC
Porosity	n	0.39
Permeability [m/s]	$k_v = k_h$	4.10 ⁻¹²
Fluid dynamic viscosity [Pa.s]	μ	10 ⁻³
Liquid compressibility coefficient [MPa-1]	Xfl	5.10-4

Table 1 : PC clay hydraulic characteristics



Thermal characteristics		PC
Thermal conductivity [W/(mK)]	λ	1.35
Volumetric heat capacity [MJ/(m ³ .K)]	Cv	2.84
Solid thermal expansion coefficient [K-1]	Иs	10 ⁻⁵
Liquid thermal expansion coefficient [K-1]	αw	3.10-4

Table 2 : PC clay thermal characteristics

The liner is supposed to be elastic. Here are its thermo-hydro-mechanical characteristics:

Liner properties		PC
Young's elastic modulus [GPa]	Е	50
Poisson's ratio [-]	υ	0.2
Thickness [cm]	е	30
Porosity [-]	n	0.1
Permeability [m/s]	k _v = Kh	4.10 ⁻¹⁰
Thermal conductivity [W/(mK)]	λ	1.5
Volumetric heat capacity [MJ/(m ³ K)]	Cv	1.8
Solid thermal expansion coefficient [K-1]	$lpha_{ m S}$	1.2*10 ⁻⁵
Liquid thermal expansion coefficient [K-1]	$lpha_{W}$	3.10-4

Table 3 : Liner properties

Note : The liner is watertight, but, for the scoping calculation, in order to be able to take into account the different hydraulic conditions, we propose to consider that the liner is permeable.

Interface elements properties :

Thermal flow interface element properties		
Porosity	no	0.3
Transverse transmissivity	Tī_c	10 ¹⁰



Hydraulic flow interface element properties

Porosity	no	0.3
Transverse transmissivity	Тн_с	10-8
Table 4 : Interface element properties		

2.3 INITIAL CONDITIONS

The clay formation around the gallery is considered as homogeneous and isotropic. However, the initial stresses are supposed to be lithostatic and anisotropic ($\sigma_v = \rho.g.z, \sigma'_H = K_0 \sigma'_v$), ρ is the material specific mass, *g* the gravity acceleration and *z* the depth). In addition, the modelling zone is supposed to be sufficiently deep so that the variation of the stresses and pore pressure with depth is neglected. The formation is supposed to be completely saturated. Initial conditions to be considered are listed in table 5:

Initial state		РС
Total strassas [MDa]	σ_{H}	4.05
Total successes [will a]	σ_v	4.5
Pore pressure [MPa]	$P_{w\theta}$	2.25
Effective stresses [MPa]	σ'_{H}	1.80
	σ'_v	2.25
Temperature [°C]	T_{0}	16

Table 5 : Initial state - stresses, pore water pressure and temperature

2.4 BOUNDARY CONDITIONS

Mechanical boundary conditions are imposed such as:

- The u_v displacements are fixed on the boundaries AC
- The u_x displacements are fixed on the boundaries BE
- The normal stress is equal to σ_H on the boundary CD
- The normal stress is equal to σ_v on the boundary ED

Hydraulic boundary conditions are imposed such as:

- The boundaries AC and BE are impermeable
- P_w is fixed equal to P_{w0} on the boundaries CD and DE

Thermal boundary conditions are imposed such as:

- The boundaries AC and BE are adiabatic
- T is fixed equal to T_0 on the boundary CD and DE





To simulate the excavation, the total radial stresses and the water pressure at the tunnel face (AB) decrease linearly to 100 kPa (so that the effective stresses are equal to zero). The convergence of the gallery is controlled and the liner is placed to allow a given convergence α^{exc} . At the end of the excavation, the contact is realized between the soil and the liner. The excavation is then followed by a one-year open drift period during which the liner face GF is supposed to be under drained conditions (the pore water pressure is fixed to be equal to the atmospheric pressure).

During the heating phase, various boundary conditions could be imposed on the liner inner face GF. For this modeling, the following boundary conditions are considered: a given decreasing heat flux and a hydraulic condition (drained).

2.5 THERMO-HYDRO-MECHANICAL SOLICITATIONS

Here is the general definition for the simulations where t^{exc} is the end time of excavation, t^{liner} the end time of the liner installation, $t^{drainage}$ is the open drift time after construction of the gallery during which the gallery is considered to be under drained or dripping conditions.

• Excavation (t^{exc}):

Excavation of the gallery is realized within $t^{exc} = 3$ days by reducing linearly the total radial stresses and the water pressure at the tunnel surface (AB) at the atmospheric pressure 0.1 MPa (so that the effective stresses are equal to zero).

• Liner installation (t^{liner})

The liner allows a given convergence α^{exc} before contact with the host rock. Once the contact is realized, an interface element allows hydraulic and thermal fluxes between the host rock and the liner. The liner is installed just after excavation

The hydraulic boundary condition at the liner inner surface GF corresponds to a drained condition during all the modeling.





• Heating $(t^{heat} = 1000 \text{ years})$

Canisters are placed in the gallery and a decreasing heat flux is given out at the liner inner surface GF (liner) or at the gallery wall AB (no liner). The simulation duration is 1000 years. During this phase, the hydraulic boundary conditions (corresponding to drained conditions) are imposed on the liner inner face GF (liner) or at the gallery wall AB (no liner).

2.6 THERMAL SOURCE THERMS

Concerning the thermal source terms for the scoping calculations of PC clay, we propose to study only the VHLW waste. The heat fluxes of these wastes in function of the time after their production are given in the figure 3.



Figure 3 : Time evolution of heat flux (W/tHM) of VHLM wastes after their production (PC case) $\$

The heat production of the wastes is calculated thanks to the following equation:

$$Q = \sum_{i} A_{i} e^{-\lambda_{i} t}$$

where Q is expressed in W/tHM and t in years.

Note : tHM (tonnes Heavy Metal) refers to the initial mass of the wastes.

For the Vitrified High Level Waste (VHLW):

 $\begin{array}{lll} A_1 = 5021 & \lambda_1 & 0.3894 \\ A_2 = 1205 & \lambda_2 & 0.02458 \end{array}$





$A_3 = 27.04$	λ_3	$1.63 \ 10^{-03}$
$A_4 = 0.7576$	λ_4	$6.546 \ 10^{-05}$
$A_5 = 0.1$	λ_5	0

Three cases of degradation before storage in the gallery are considered :

- After 50 years of storage (Reference case);
- After 30 years of storage;
- After 80 years of storage.

Totally, we have 3 thermal source terms to be applied directly on the gallery liner.

For the scoping calculations, we need to express these thermal source terms in terms of linear thermal load density (W/m). The conversion depends on the repository designs. For PC case, we consider the Supercontainer designs for VHLW: 1.3 tHM/canister and 2 canisters/4.2 m.

This gives the linear thermal density of 239.62 W/m after 50 years, 381.94 W/m after 30 years and 122.38 W/m after 80 years of storage.



3 EXERCISE DEFINITION

For this exercise, we propose you to model the scoping calculation described before. For time reasons, all the files needed for the modeling were prepared and installed on each computer. THM modeling implies different physical complex phenomena. In order to evidence each physic, we propose to proceed step by step and to study first the thermal problem, then the thermo-hydraulical problem and finally the THM problem. For that purpose, you will use the finite element code Lagamine, which description could be found in the 'User manual for Lagaprogs 5.1'.

Running Lagaprogs, a presentation window will appear and wait for a user name. You have to enter 'TIMODAZ' as user name and the Lagaprogs platform is then available. We have already defined a project made of three different simulation cases corresponding to the steps of the exercise. You can thus open the project 'Scoping' and the simulation case 'Thermal'. You will observe that different files are already present in the directory and referring to the 'User manual', you are able to run some modeling.

The objective of this exercise is not to teach you how to run a FE model from A to Z but to allow you to obtain some results to different physical problems. With these results, you are supposed to understand what could append around a nuclear waste disposal and what the coupling effects between the different phenomena are. For that purpose, you will use the postprocessing code GID and the results files that are generated by the code (IPN, IPE files whose structure is described in the appendix of the User Manual). Taking into account the fact that there still exist uncertainties on some parameters (for example, the thermal conductivity of the PC), some parametric sensitivity studies will be proposed too.

3.1 THERMAL PROBLEM

In the available data files (ScopingT.lag and heatex.dat), we do not consider the concrete liner and the heat flux produced by the VHLW is applied on the cavity wall ($f^{T} = 19.068$ W/m²). After running the Lagamine you will get the IPN file, in which you can find a radial profile of temperature after 1 year, 10 years, 100 years, 1000 years and 2000 years.

- Analyze the results.
- Study the influence of the thermal conductivity (1.5 W/mK).
- Study the influence of the time after which the wastes are stored in the gallery (30 y or 80 y).

3.2 THERMO-HYDRAULICAL PROBLEM

This modeling is composed of two parts corresponding to some files: Part 1 the excavation (ScopingTH_1.lag and excavationex.dat) and Part 2 Heat production (ScopingTH_2.lag and THex.dat). We do not consider the concrete liner and the heat flux produced by the VHLW is applied on the cavity wall ($f^{T} = 19.068 \text{ W/m}^{2}$).

After running the Lagamine for the first step, you will get the IPN file, in which you can find a radial profile of water pressure after 1 day, 2 days, 3 days, 15 days and 1 year.

Before starting the second step, you need to transfer the results of ScopingTH_1.f03 in the file ScopingTH_2.f03 (See section 3.14 in the User manual). After this second step, you will get the IPN file, in which you can find a radial profile of temperature and water pressure after 2 years, 11 years, 101 years, 1001 years and 2001 years.



- Analyze the results.
- Show the evidence of coupling effects during step 2.
- Do some sensitivity analysis.

3.3 THM MODELLING

This modeling is composed of two parts corresponding to some files: Part 1 the excavation (ScopingTHM_1.lag and excavationex.dat) and Part 2 Heat production (ScopingTHM_2.lag and THex.dat). We do consider the concrete liner and the heat flux produced by the VHLW is applied on the liner wall ($f^T = 23.687 \text{ W/m}^2$).

After running the Lagamine for the first step, you will get the IPN file, in which you can find a radial profile (at Y = 0) of displacement and water pressure after 1 day, 2 days, 3 days, 15 days and 1 year. You will get also the IPE file, in which you can find a radial profile (at Y = 0) of the effective stress after 1 day, 2 days, 3 days, 15 days and 1 year.

Before starting the second step, you need to transfer the results of ScopingTHM_1.f03 in the file ScopingTHM_2.f03. After this second step, you will get the IPN file, in which you can find a radial profile of displacement, temperature and water pressure after 2 years, 11 years, 101 years, 1001 years and 2001 years. You will get also the IPE file, in which you can find a radial profile (at Y = 0) of the effective stress after 2 years, 11 years, 101 years and 2001 years.

- Analyze the results.
- Show the evidence of coupling effects.
- Do some sensitivity analysis.

