Inria Project Lab C2S@Exa
Computer and computational sciences at exascale
Radioactive waste management application

Numerical simulation at ANDRA

Context, goals, needs, and issue for IPL C2S@Exa

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General overview of Andra (1/2)

Andra, the French National Radioactive Waste Management Agency, was instituted by law in 1991 as a public industrial and commercial establishment (EPIC). It is:

- **independent** from the waste producers
- placed under the **supervision of the ministers** in charge of Research, Energy and the Environment
- responsible for the **long-term management** of all radioactive waste produced in France
- it involves about **550 employees**

The *Planning Act of 28 June 2006 concerning the sustainable management of radioactive materials and waste provides the framework for its action.*

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General overview of Andra (2/2)

One main mission

- Find, implement and ensure safe management solutions for french radioactive wastes, in order to protect present and future generations from the the risk of these wastes.

Several activities

- Operate and monitor existing storage centers
- Study and design disposals for waste awaiting the creation of a suitable center
- Collect radioactive waste objects held by “individuals”
- Remediation of sites polluted by radioactivity
- List all materials and radioactive waste produced in France (volumes, location, estimated volume)
- Inform the public of all radioactive wastes and their management
- Disseminate its expertise abroad

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Location of ANDRA facilities

Classification of radioactive waste

<table>
<tr><th>Half-life / Activity</th><th>Very short life
< 100 days</th><th>Short life (SL)
< 31 years</th><th>Long life (LL)
> 31 years</th></tr>
<tr><td>Very low level (VLL)</td><td rowspan="4">Management through in situ radioactive decay</td><td colspan="2">Surface disposal at CSTFA (Aube District)
Recycling systems</td></tr>
<tr><td>Low level (LL)</td><td rowspan="2">Surface disposal at CSFMA (Aube District) , except for certain tritiated waste and sealed sources</td><td>Under study pursuant to Art. 4 of Planning Act of 28 June 2006.
Project for shallow disposal.</td></tr>
<tr><td>Intermediate level (IL)</td><td>Under study pursuant to Art. 3 of Planning Act of 28 June 2006. Project for a deep reversible repository.</td></tr>
<tr><td>High level (HL)</td><td colspan="2">Under study pursuant to Art. 3 of Planning Act of 28 June 2006.
Project for a deep reversible repository.</td></tr>
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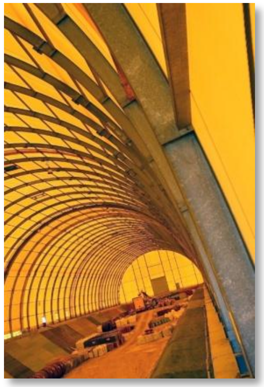
Two operating surface-disposal facilities in the Aube District

➢ The **Disposal Facility for LIL Waste** (CSFMA) opened in 1992. Located in Soulaines (Eastern France), it is designed to accommodate 1 million cubic metres of LL/IL SL waste, consisting mostly of NPPs' operational and maintenance waste. Filled at 24.5% with 60 years of operation to go.

➢ The **Disposal Facility for VLL Waste** (CSTFA) opened in 2003 at Morvilliers. It is used to dispose of 650,000 m³ of VLL waste resulting from the dismantling of basic nuclear installations. Filled at 27% with 15 years of operation to go.



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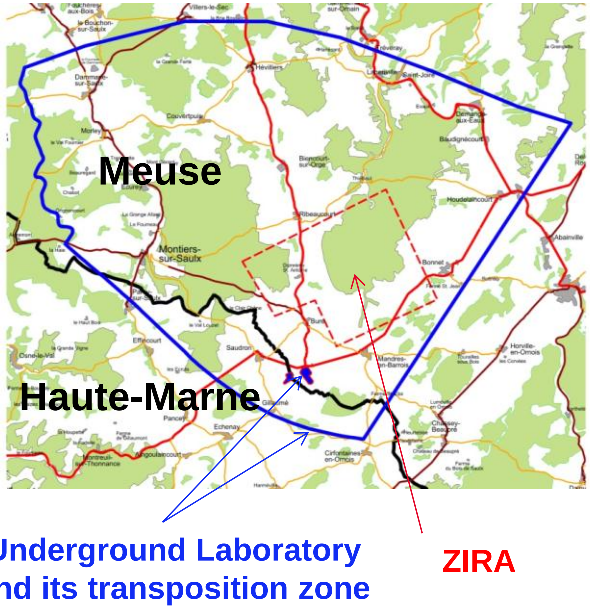
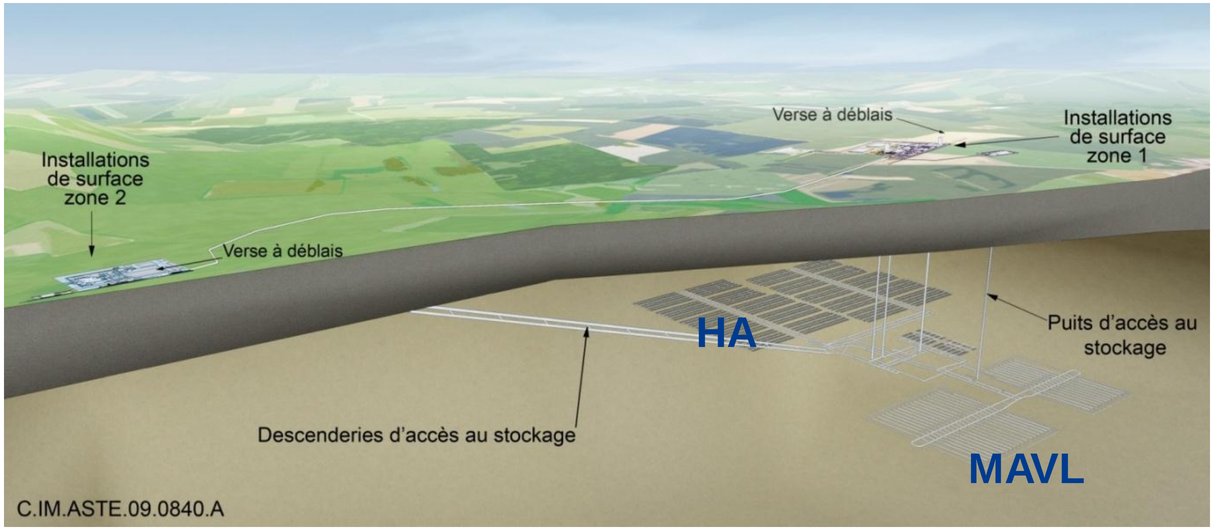
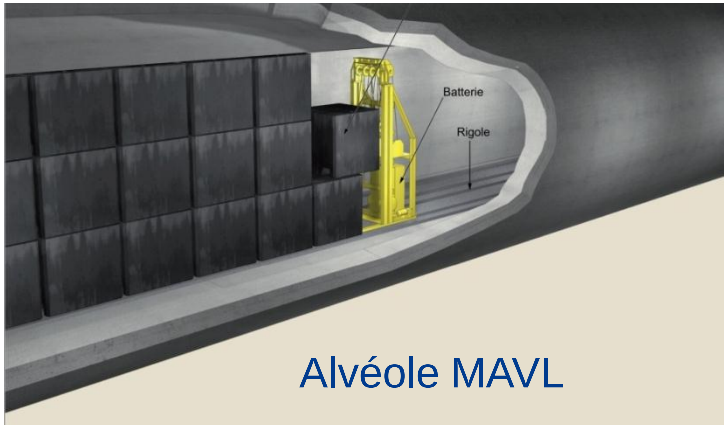
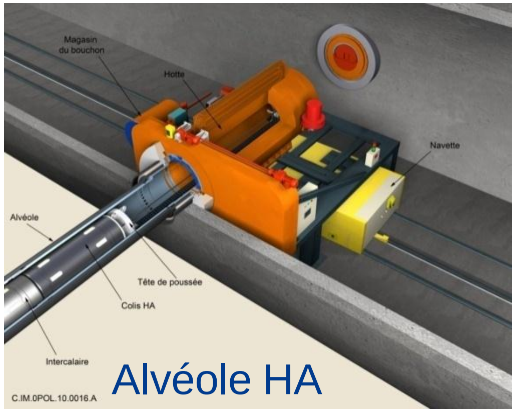
The Cigéo (Industrial Geological Waste Repository) constitutes a non-typical INB to be built underground and to remain in operation for more than 100 years









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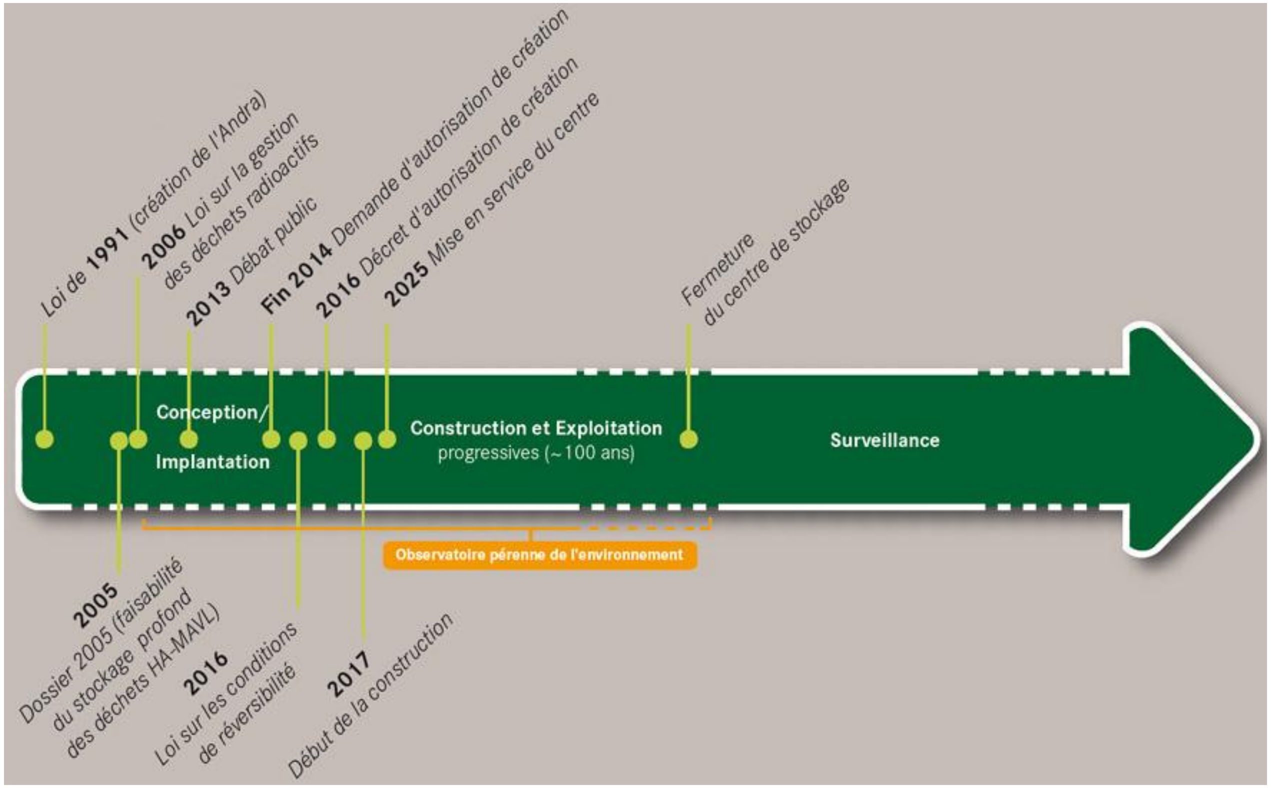
Schedule of the Cigéo Project

In late 2009, Andra submitted proposals to the government regarding the implementation and design of the repository.
The project is entering in the definition and construction phases of the industrial geological repository ("Cigéo").

Pursuant to the *Planning Act of 28 June 2006*, the three major objectives of the project are now as follows:

- to obtain the authorisation to create a repository on the basis of a robust application to be submitted in 2015
- subject to authorisation, to build the first necessary structures for commissioning in 2025

The French project will be the world's first facility of that type to be built in clay.



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Safety issues

In its capacity as contracting owner and INB operator, Andra is responsible for design choices and their implementation, which are bounding over the long term.

Compared to existing facilities, the underground repository includes specificities that do not allow for restricting the task to a simple transposition of practices :

- Demonstration of the long-term safety of the facility over 1 million years
- For operational safety: management of the co-activity between underground work at a depth of 500 m and nuclear operation
  - ☐ *No fire reference system (INB, tunnel) is applicable as such.*

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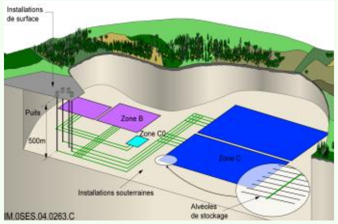
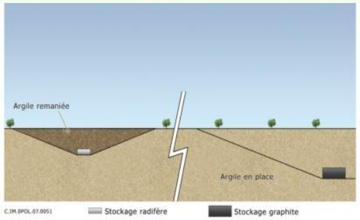
Numerical simulation at Andra : a tool to fulfill issues

Disposals/Projects

Cigeo Project
High-Level and intermediate-level long-lived radwaste
Deep geological reversible disposal



FAVL Project
(Low-level and long lived radwaste)
(Radifer)
Surface and low-depth repository



Surface centers
(Low and very low-level radwaste)
CSFMA, CSTFA
centre Manche

Domain of application

Modeling/Numerical simulation at Andra: a preferential tool for

1. Representation of phenomenological evolution (PARS method)

2. Choice of concept and design

3. Performance/Safety Assessment

4. Design and interpretation of experiments, in particular in URL

5. Sitting

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Main missions of Performance Assessment Department (1/2)

Description/quantification of phenomenological behavior of **disposal components scale and geological environment** (*operating and post-closure period*)

- Integration of scientific and basic knowledge objects in a logic {components, physical process, space, time}
- Conceptualization and Quantification of Thermo-Hydro-Mechanics-Chemical-Radiological “states”

Assess performance of disposal system in quantitative safety analysis context

- Integration of phenomenological knowledge in logic {objects / components, process, space, time, safety functions}
- Quantification of indicators related to the release and migration of radionucleides
  - Flow, molar rates, concentrations, transfer times, attenuation (input / output) of each component, Peclet numbers , .., doses
- Achievement of safety calculations
  - Physical and numerical conceptualization done by Andra
  - Numerical simulations performed both by Andra and sub-contractors

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Get/develop tools able to represent multi-physics coupling over large time and space scales (continuous improvements of software development since 2000)

- Three main areas of R & D:
  - ☐ simulation of physical processes
    - + *Implementations of multi-physics couplings*
  - ☐ numerical methods and HPC
    - + *Parallelism,*
    - + *Domain decomposition methods space / time*
    - + *Robust numerical methods*
    - + *Efficient algorithms for grid generation*
  - ☐ uncertainty and sensitivity analysis methods

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Modeling/Simulation: state of the art on softwares used by Andra

Single-phase flow saturated /unsaturated (Richards)
- Porflow
- Traces
- Feflow
- Modflow
- GroundWater

Solute transfer
- Porflow
- Traces
- Feflow
- MT3D
- GroundWater

Two-phase flow
- Tough2_MP (//)
- Code_Bright

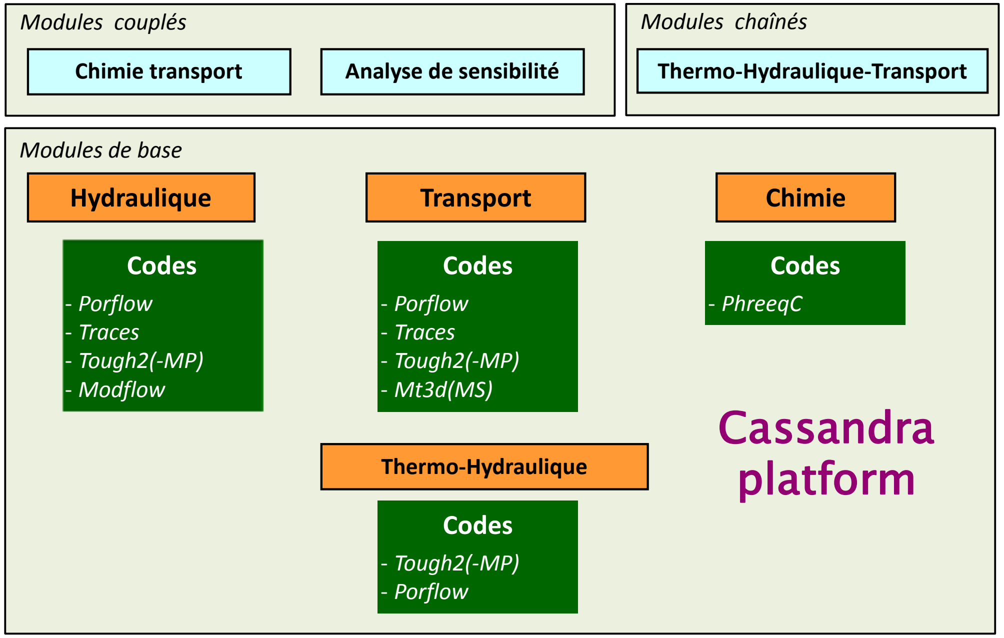
ToolBox
- Comsol

Chemistry /transport
- PhreeqC
- Phast (//)
- ToughReact
- CrunchFlow
- *(GRT3D)*

Geomechanics
- Code_Bright (porous media)
- Castem (structures)

Specific tools used by sub-contractors : Qpack, Ansys, Geoan, Hydrogeosphere, Hytec, …

Pre/post-Processing
- Mailleurs : Map/Mappy/Gambit/ICEM
- **Visualisation** : Tecplot3D, Surfer, Grapher, Xmgrace,…



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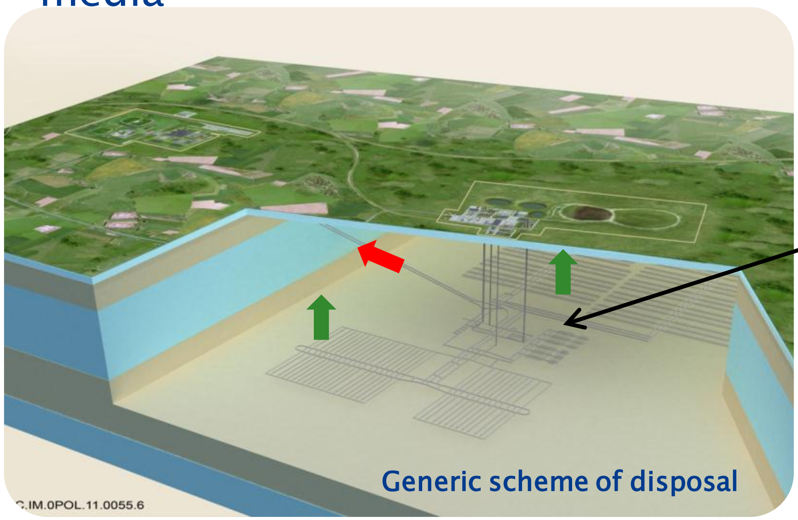
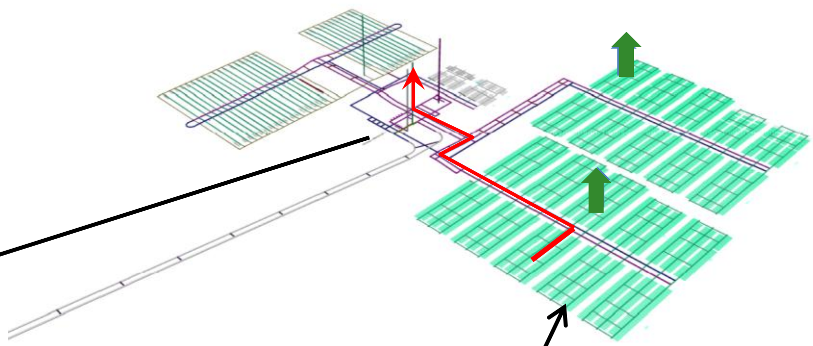
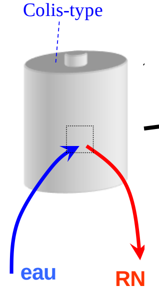
Context

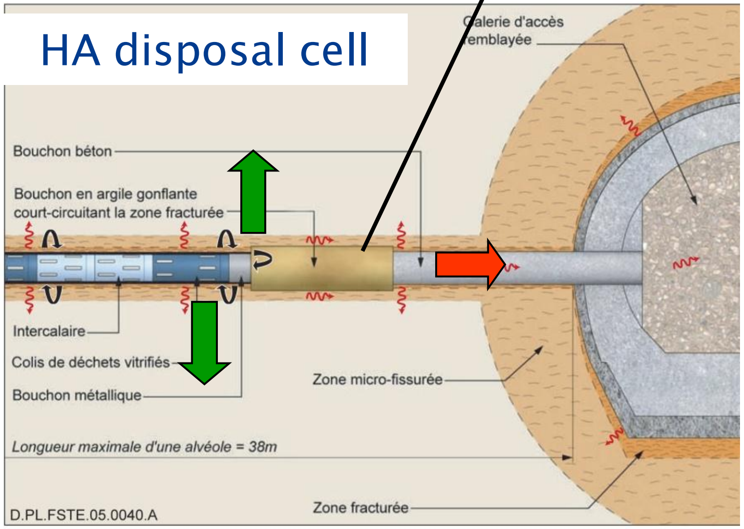
- Long-term performance and safety assessment for Cigéo disposal (can also be applied for CSA center)
- Hydraulic and migration of solute transfer from the waste packages to geological media



Generic scheme of disposal







HA disposal cell

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Issues/Goals

- Reference « Single » including all details from waste packages scale to multi-layers geological system, managing following difficulties :
  - 6 orders of magnitude of space scale (from decimeter to pluri-kilometric)
  - Many caracteristic time scales (clay layer, surrounding formations, repository structures)
  - Contrasts of
    - hydrodispersive input data (up to 4/5 orders of magnitude of permeability)
    - Process of transfer (advection/diffusion), with/without any sorption
- Get the best information about behaviour of nuclides in the system
  - Pathways (space/time)
  - Attenuation/retardation of each component
  - Managing « easily » uncertainties
  - Reference case (as realistic as possible)
    - Reference for simplifications (quantifications of approaches for more simple cases)
- To get for the future **a « reference » tool**
  - which is available and sustainable
  - Which is no more only a commercial one
  - Which can include « easily » all relevant numerical methods
- To get a powerful tool which is likely to be used for great problems (huge size) in several applications (Cigéo, CSA, ...)

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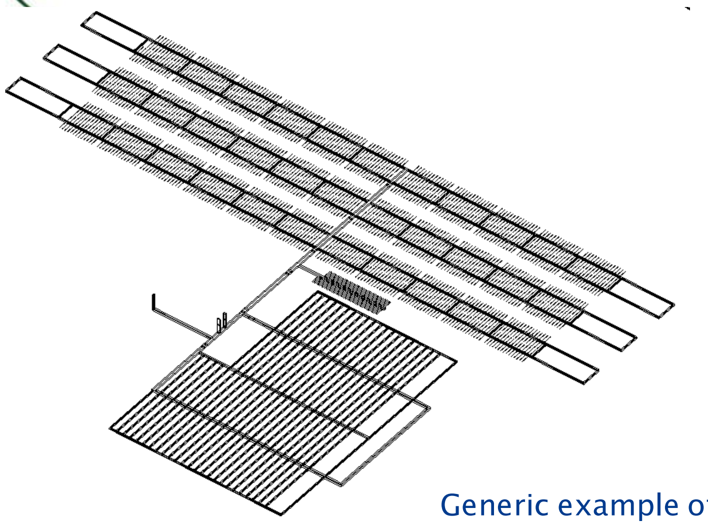
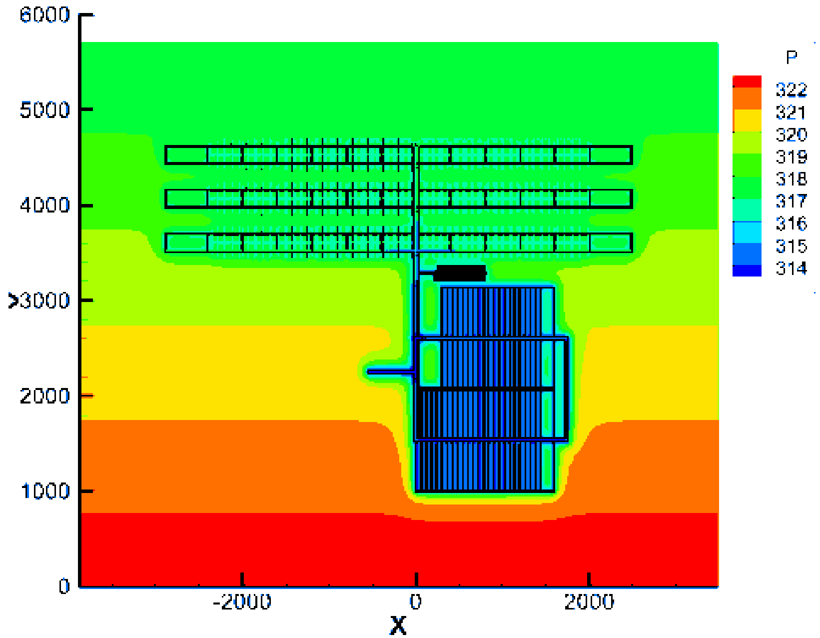


Generic example of results



Up-to-date calculation with Porflow

- 10 millions cells in structured mesh, including all disposal cells and zone
- Many simplifications
  - *Only clay layer considered*
  - *A few cells (grid) per « disposal cell »*
  - *Drifts/galleries gathered*
  - *Shafts gathered*
  - *Macro-components*
- « Rectangular » approach
  - *Disposal cell*
  - *Same thickness of clay layer*
  - *…*
- Several days of computing
  - *Limit for sensitivity analysis*

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Hydraulique

Équation de continuité du fluide

+

Équation de Darcy $\vec{U} = -K\vec{\nabla}h$

Équation « diffusivité nappe captive »

$$div\left(\overline{\overline{K}}\vec{\nabla}h\right) = S_S \frac{\partial h}{\partial t} + q$$

Solution en régime permanent

$$div\left(\overline{\overline{K}}\vec{\nabla}h\right) = q$$

$\vec{U}$	champ de vitesse de Darcy	[L/T]
q	débit par unité de volume de fluide apporté ou prélevé	$[T^{-1}]$
K	perméabilité	$[L.\ T^{-1}]$
h	charge ou hauteur piézométrique	[L]
Ss	coefficient d'emmagasinement spécifique	$[L^{-1}]$

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Transfert des Radionucléides en solution en milieu poreux saturé (1/3)

$$\omega R_i \frac{\partial C_i}{\partial t} = div\left(\overline{\overline{D}}\,\vec{\nabla} C_i - C_i \vec{U}\right) - \omega \lambda_i R_i C_i + \omega \sum_{j \in I} \sigma_{ji} \lambda_j R_j C_j + S_i + \rho.\omega.J_i$$

avec

ω	porosité	[1]
R_i	coefficient de retard du RN i dans le milieu	[1]
C_i	concentration en solution du RN i	$[mol.L^{-3}]$
$\overline{\overline{D}}$	tenseur de dispersion-diffusion (cf. ci-après)	$[L^2.T^{-1}]$
$\vec{U}$	champ de vitesse de Darcy	$[L.T^{-1}]$
λ_i	constante de décroissance radioactive du RN i	$[T^{-1}]$
I	ensemble des antécédents du radionucléide i	
σ_{ji}	fraction du radionucléide j se désintégrant en radionucléide i	[1]
S_i	terme source du radionucléide i	$[mol.L^{-3}.T^{-1}]$
ρ	masse volumique de l'eau interstitielle	$[M.L^{-3}]$
J_i	terme d'échange avec la phase solide	$[mol.M^{-1}.T^{-1}]$

$$\overline{\overline{D}} = De.\delta_{ij} + \alpha_T.\left|\vec{U}\right|.\delta_{ij} + \frac{(\alpha_L - \alpha_T).u_i u_j}{\left|\vec{U}\right|}$$

De	coefficient de diffusion effective	[L².T-1]
α_L	dispersivité longitudinale	[L]
α_T	dispersivité transversale	[L]

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Transfert des Radionucléides en solution en milieu poreux saturé (2/3)

Prise en compte de la **rétention géochimique** selon deux processus (1/2)

1. La Sorption ,via un coefficient de retard [R]

Le coefficient de distribution [Kd] est relié au coefficient de retard [R] par l'équation :

- sorption linéaire réversible instantanée dans la plupart des cas $R = 1 + \frac{1-\omega}{\omega} \rho \; .K_d$

avec :

Kd	coefficient de distribution entre l'eau et la roche pour le radionucléide	$[L^3. M^{-1}]$
ρ	masse volumique des particules solides (densité de grain)	$[M. L^{-3}]$
ω	porosité	[-]

La quantité sorbée se calcule alors comme : $C_i^{sorbé} = \mathrm{K}d_i.C_i$

- sorption qui suit une isotherme (ex : Langmuir) pour certains cas $R_i = 1 + \left(\frac{1-\omega}{\omega}\right)\rho \frac{A_i}{C_i + B_i}$

avec Ai, Bi constantes définissant la loi de Langmuir

La quantité sorbée se calcule alors comme : $C_i^{sorbé} = \frac{A_i^l.C_i}{B_i^l + C_i}$

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Transfert des Radionucléides en solution en milieu poreux saturé (3/3)

Prise en compte de la **rétention géochimique** selon deux processus (2/2)

2. La **Précipitation** , via une limite de solubilité [Csat]

Représentée par une comparaison entre concentration en solution (C) et limite de solubilité (Csat) :

-si $C \leq Csat$, pad de création de précipités → Rn soluble

-si $C > Csat$, il y a création de précipités
- dont il faut gérer l'évolution dans le temps
- soumis aux phénomènes de décroissance et à la filiation radioactive,

→ terme source spécifique de l'équation de migration

$$J_i = \varpi_i . (Csat_i - C_i) . \delta_i$$

J_i terme d'échange avec la phase liquide (modèle linéaire) $[mol.M^{-1}.T^{-1}]$

ϖ_i constante d'équilibre entre soluté et précipité pour l'isotope i,

$Csat_i$ limite de solubilité effective pour l'isotope i (masse d'isotope par masse d'eau),

δ_i fonction corrective du transfert pour l'isotope i :

égale à 0 si et $C_l^i \leq C_{Sat}^i$ (cas soluble), égale à 1 sinon (cas précipité).

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