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Swiss Federal Nuclear Safety Inspectorate ENSI

Benchmark Calculations with COMSOL

Transport of Radionuclides through Clay and Bentonite Barriers in a Geological Repository

Manuel Lorenzo Sentis, Felix Altorfer, Martin Herfort (ENSI)
Andreas Jakob, Georg Kosakowski (PSI)
Sven Friedel (COMSOL)

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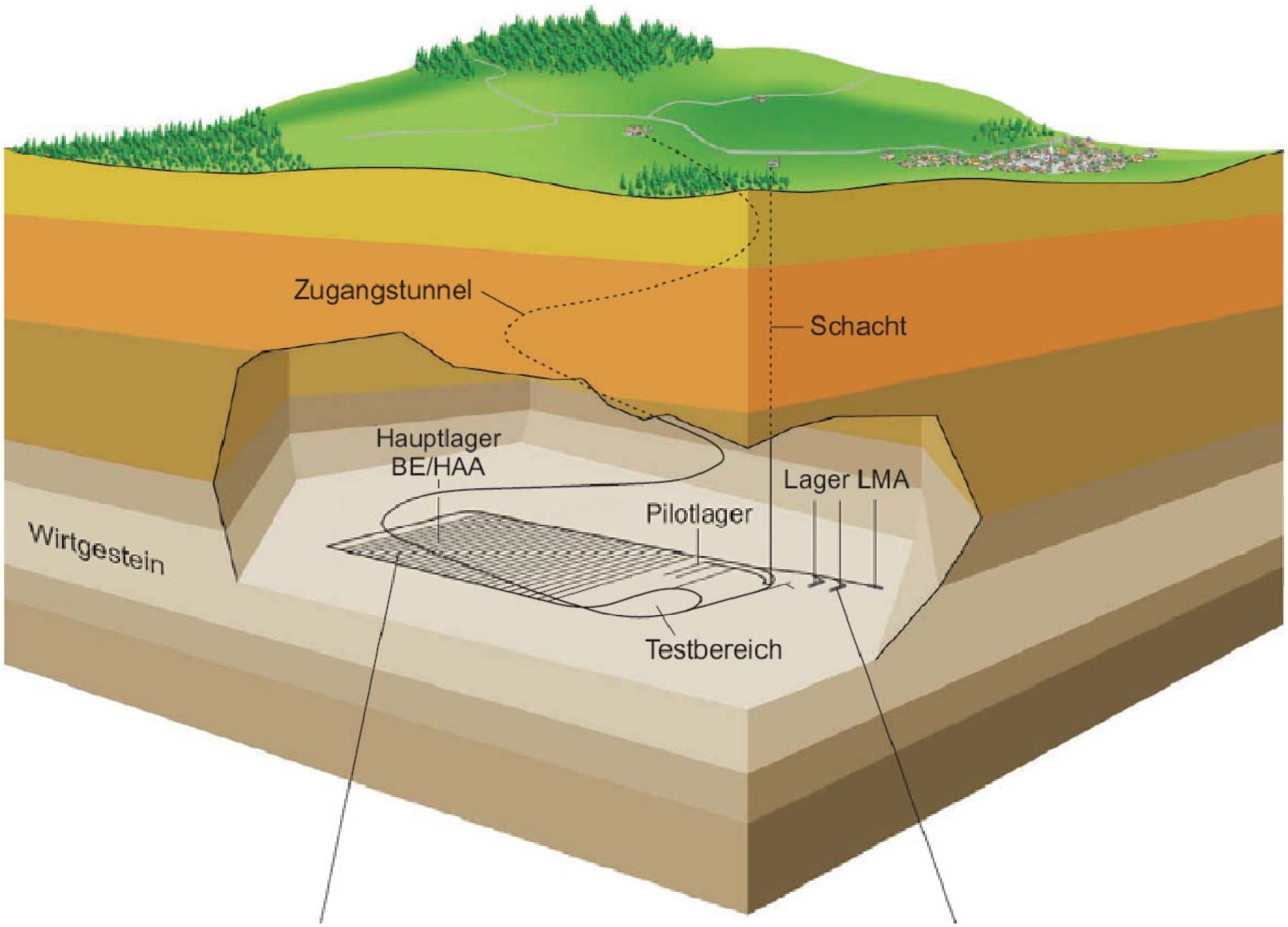
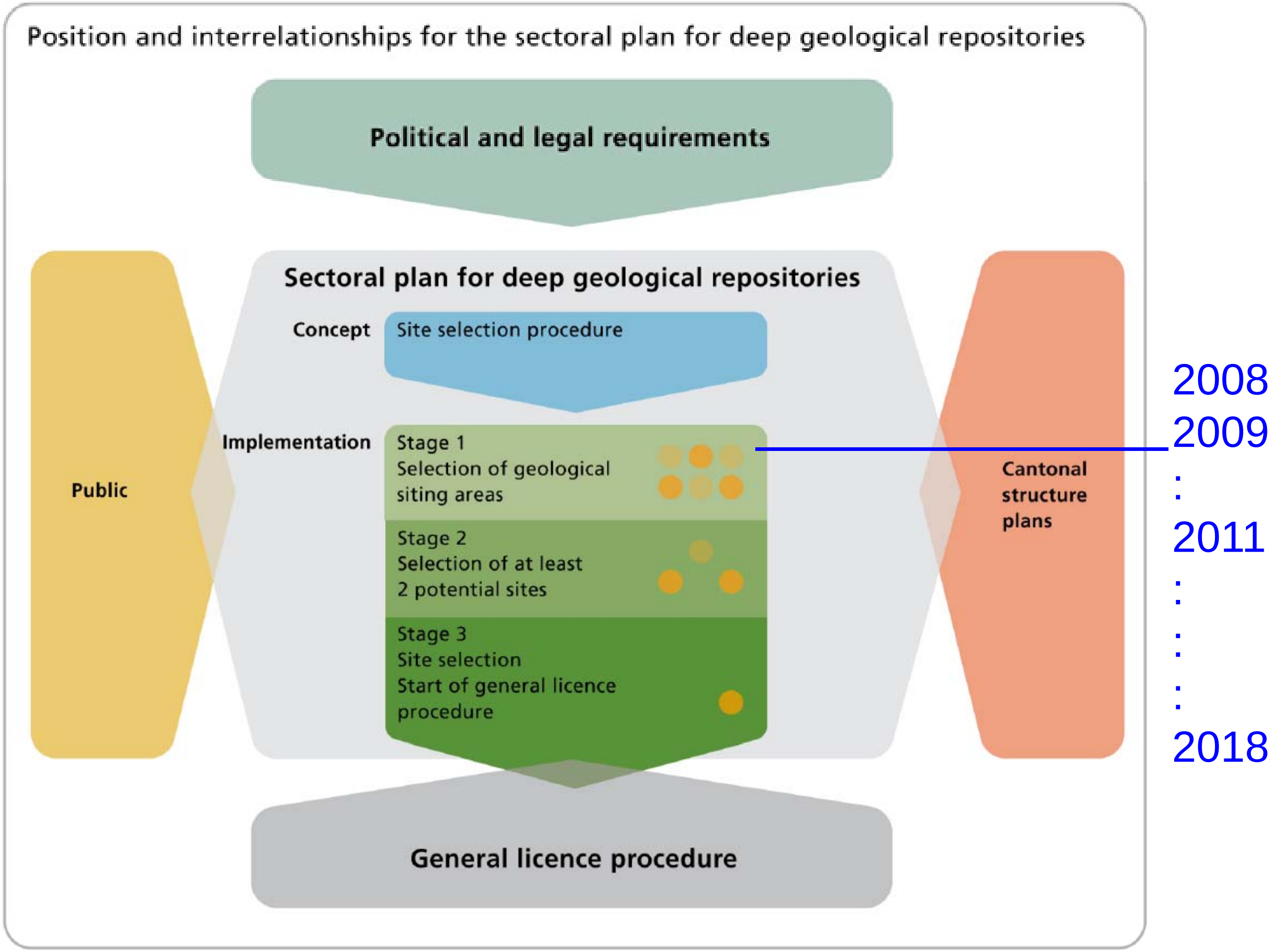
Outline

- Context of the benchmark study
- Physical problem and conceptual model
- Results
- COMSOL topics
- Conclusions

Geological Repository for Radioactive Waste Disposal



Sectoral Plan for Site Selection



Swiss Federal Nuclear Safety Inspectorate ENSI

- Supervisory authority for nuclear safety and radiation protection in nuclear facilities in Switzerland
- For Radioactive waste disposal:
  - Review of the site proposals and safety assessments submitted by the Swiss implementer Nagra
  - Independent research
- 10 scientist of different disciplines

Numerical Simulation Tools

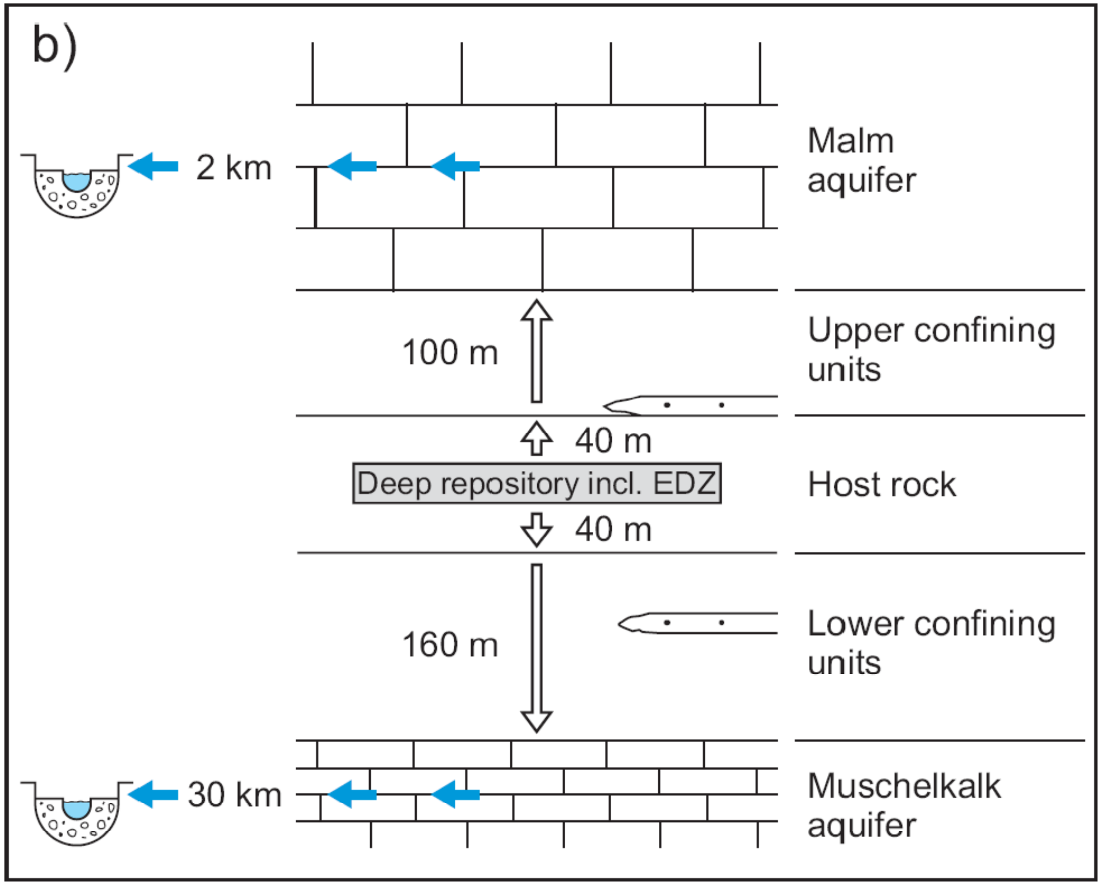
- In the past, ENSI (former HSK) developed own simulation tools (femtrac, tube)
- Today, international recognized codes like Tough2 and COMSOL are available
- These codes are not used by the implementer → cross-checking the results
- Numerical simulations will play a major role in the current site selection process

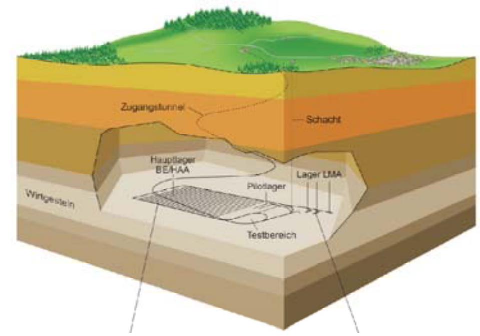
Benchmark

- Verification of the codes Tough2-EOS9nT and COMSOL
- Verification of our capabilities to use the codes
- Benchmark: Calculations of a feasibility study, performed by Nagra and repeated by PSI:

  "Demonstration of disposal feasibility for spent fuel, vitrified high-level waste and long-lived intermediate level waste" NTB 02-05 (Nagra)
- Collaboration of PSI and ENSI
- Preparation for the calculations within the sectoral plan

Simplifications: Geology





Legend:

Transport mechanism:

⇨ Mainly diffusion

Mainly advection:
- relatively large
- relatively small

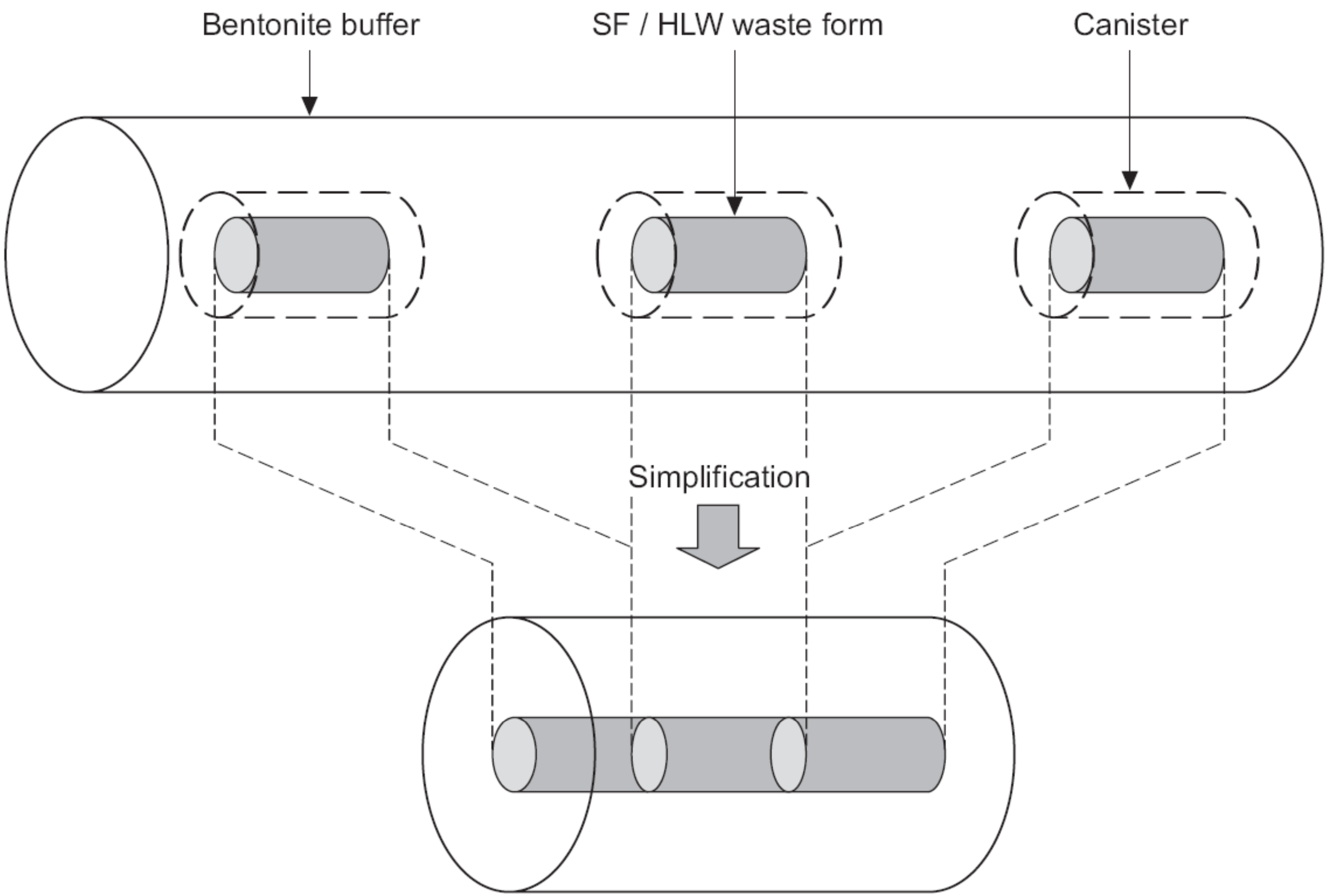
} water flows

Exfiltration area:

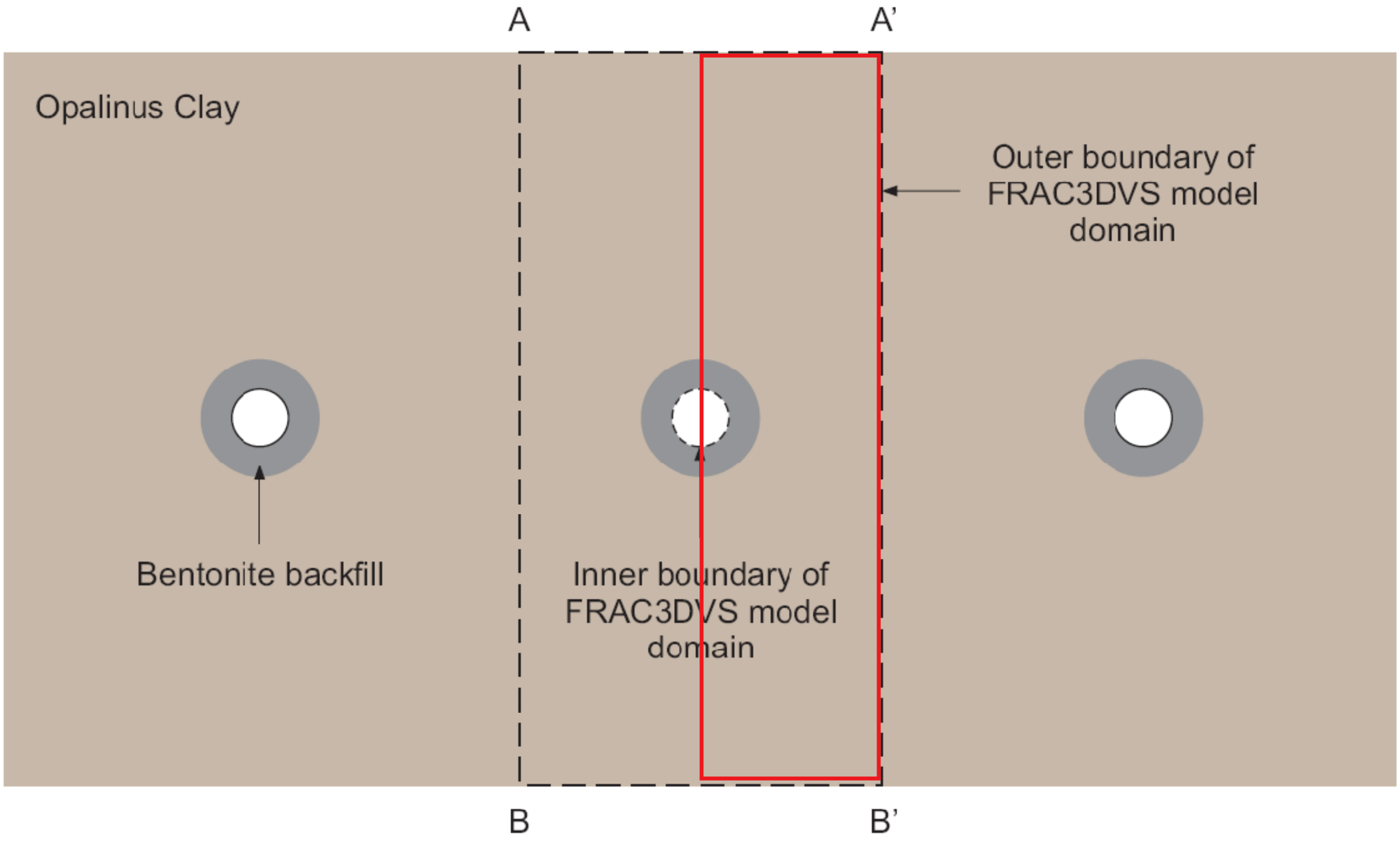
River valley with Quaternary gravels

W: Wedelsandstein
Sk: Sandsteinkeuper

Simplifications: Dimensions

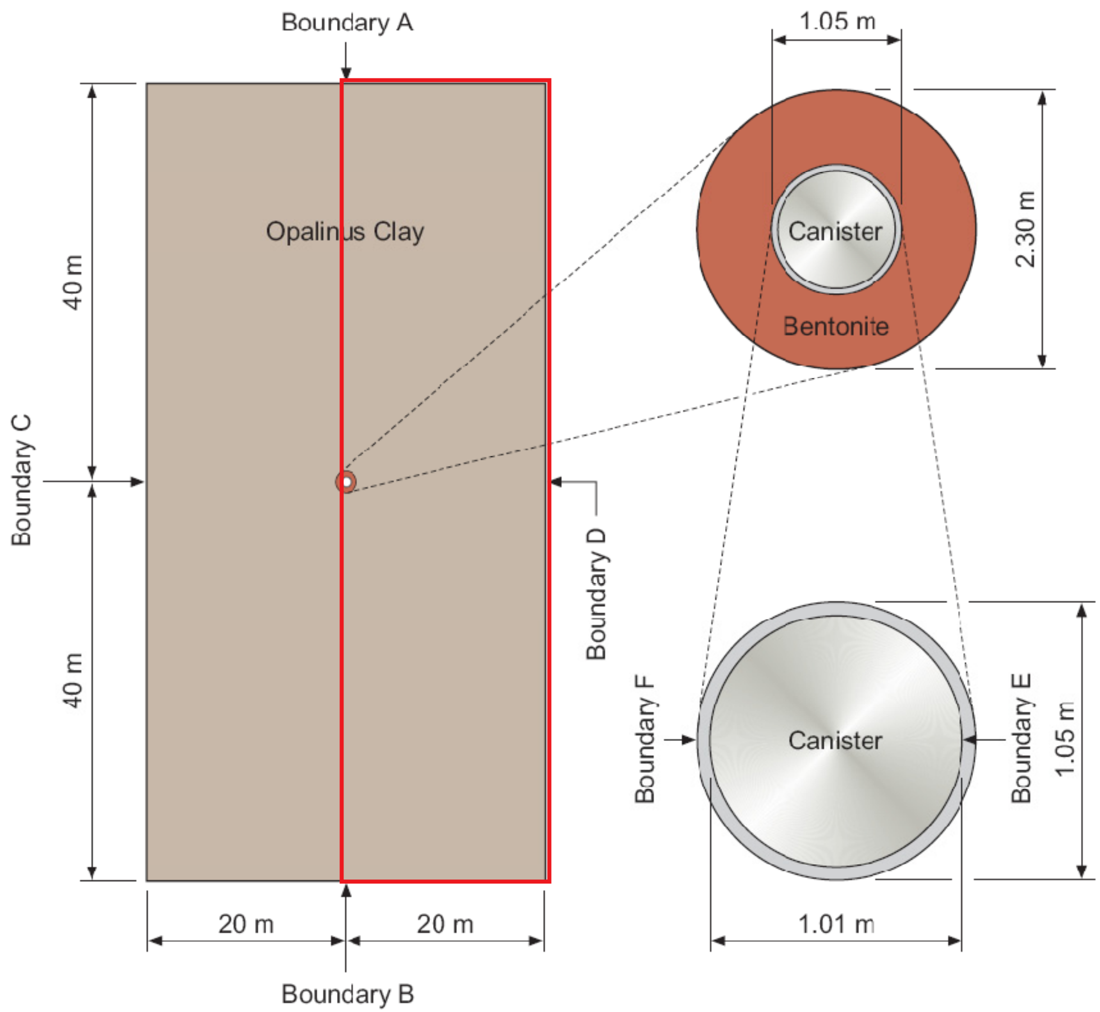


Simplifications: Symmetry



Conceptual Model

Bentonite
$K_x=K_y=1.0\cdot10^{-13}$ m/s
$K_z=1.0\cdot10^{-13}$ m/s
$\rho=2.76\cdot10^{3}$ kg/m^3



Opalinus Clay
$K_x=K_y=1.0\cdot10^{-13}$ m/s
$K_z=2.0\cdot10^{-14}$ m/s
$\rho=2.72\cdot10^{3}$ kg/m^3

Selection of Codes and Nuclides

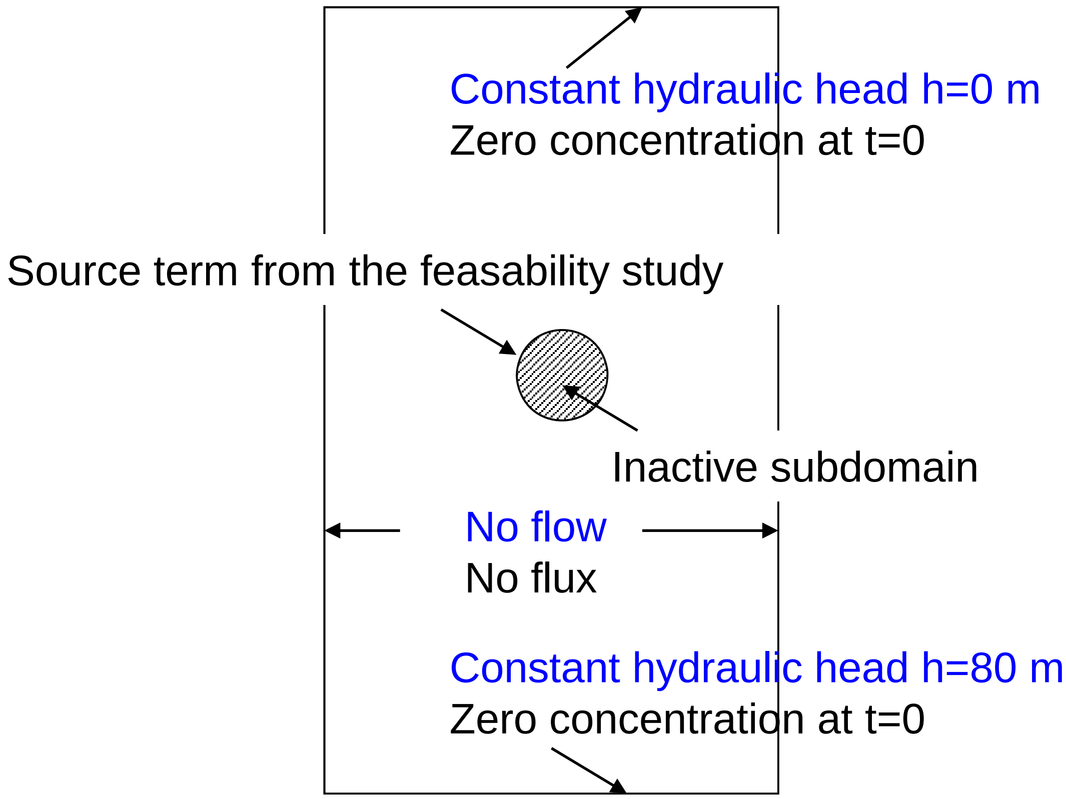
Critical Radionuclides were chosen:

- C-14
- Ca-41
- Cl-36
- I-129
- Se-79

Several Codes were used:

- COMSOL (ENSI)
- Tough2-EOS9nT (ENSI)
- Picnic (Nagra, Colenco)
- Frac3dvs (PSI)

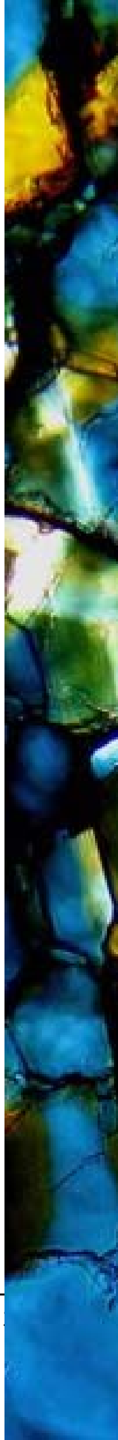
Boundary and Initial Conditions



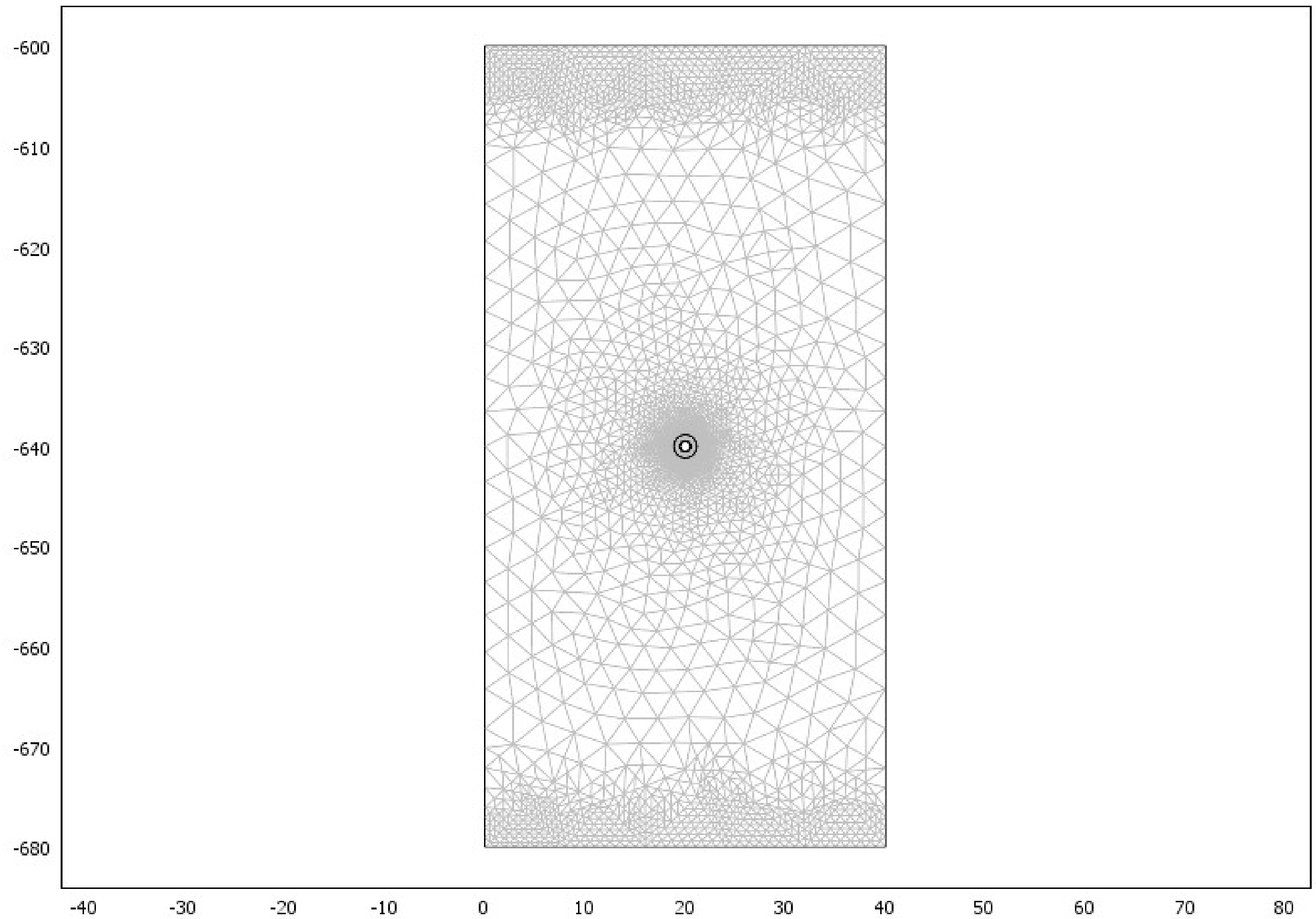
Stationary flow and transient solute transport

Radionuclides Properties

Parameter	**Unit**	**Ca-41**	**C_{org}-14**	**Cl-36**	**I-129**	**Se-79**
Molecular diffusion coefficient D_0	$m^2 a^{-1}$	$1.75\cdot10^{-2}$	$1.75\cdot10^{-2}$	$1.89\cdot10^{-3}$	$1.89\cdot10^{-3}$	$1.89\cdot10^{-3}$
Decay constant	a^{-1}	$6.73\cdot10^{-6}$	$1.21\cdot10^{-4}$	$2.31\cdot10^{-6}$	$4.41\cdot10^{-8}$	$6.3\cdot10^{-7}$
Half life $T_{½}$	a	$1.03\cdot10^{5}$	$5.73\cdot10^{3}$	$3\cdot10^{5}$	$1.57\cdot10^{7}$	$1.1\cdot10^{6}$
Bentonite	**Unit**	**Ca-41**	**C_{org}-14**	**Cl-36**	**I-129**	**Se-79**
Effective Porosity	-	0.36	0.36	0.05	0.05	0.05
Effective diffusion coefficient D_e	m^2/s^{-1}	$2\cdot10^{-10}$	$2\cdot10^{-10}$	$3\cdot10^{-12}$	$3\cdot10^{-12}$	$3\cdot10^{-12}$
Distribution coefficient for sorption K_s	$m^3 kg^{-1}$	$3\cdot10^{-3}$	0	0	$5\cdot10^{-4}$	0
Tortuosity t	-	1.0	1.0	1.0	1.0	1.0
Opalinus Clay	**Unit**	**Ca-41**	**C_{org}-14**	**Cl-36**	**I-129**	**Se-79**
Effective Porosity	-	0.12	0.12	0.06	0.06	0.06
Effective diffusion coefficient D_e	m^2/s^{-1}	$1\cdot10^{-11}$	$1\cdot10^{-11}$	$1\cdot10^{-12}$	$1\cdot10^{-12}$	$1\cdot10^{-12}$
Distribution coefficient for sorption K_s	$m^3 kg^{-1}$	$1\cdot10^{-3}$	0	0	$3\cdot10^{-5}$	0
Tortuosity t	-	0.15	0.15	0.278	0.278	0.278

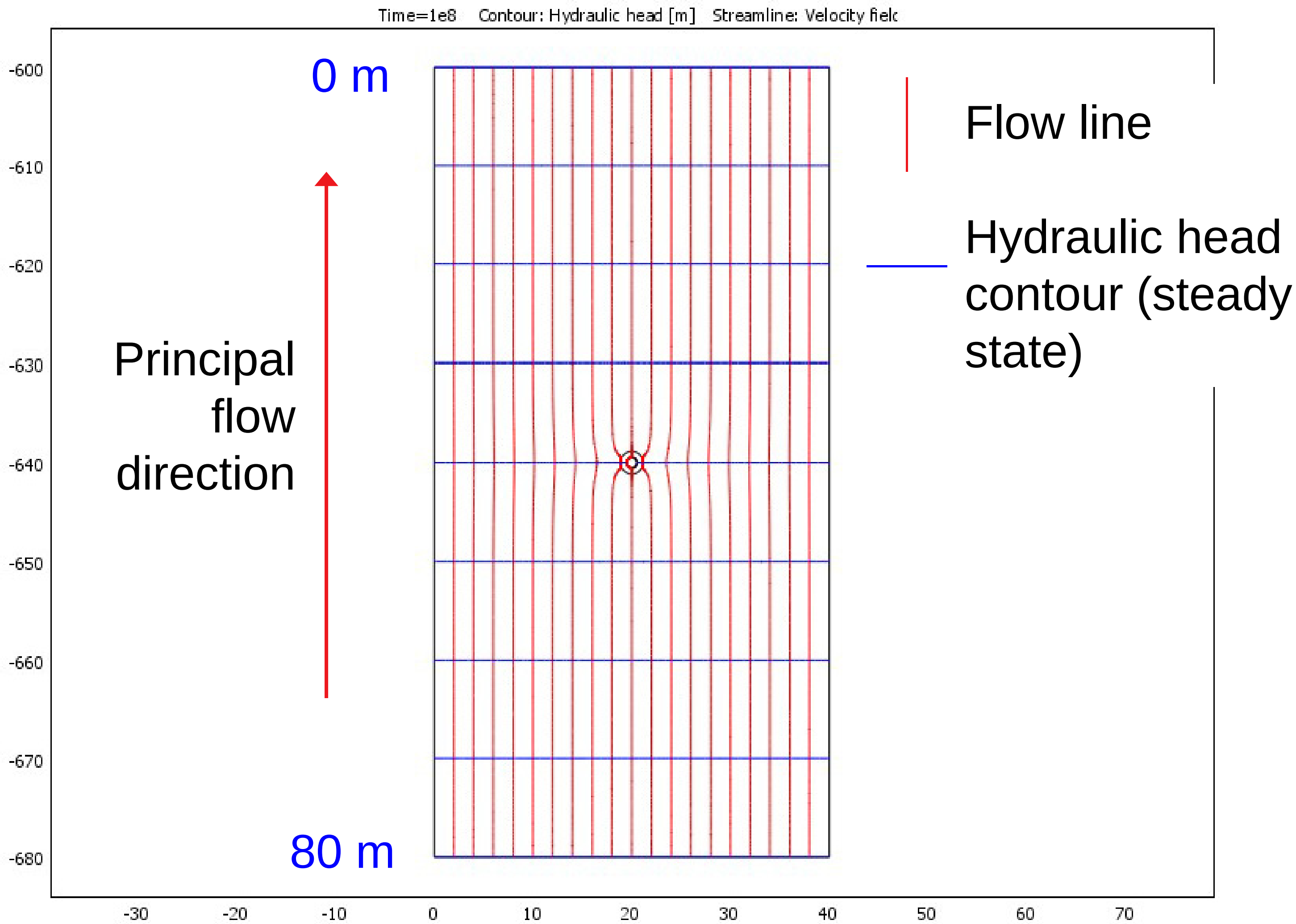


Mesh

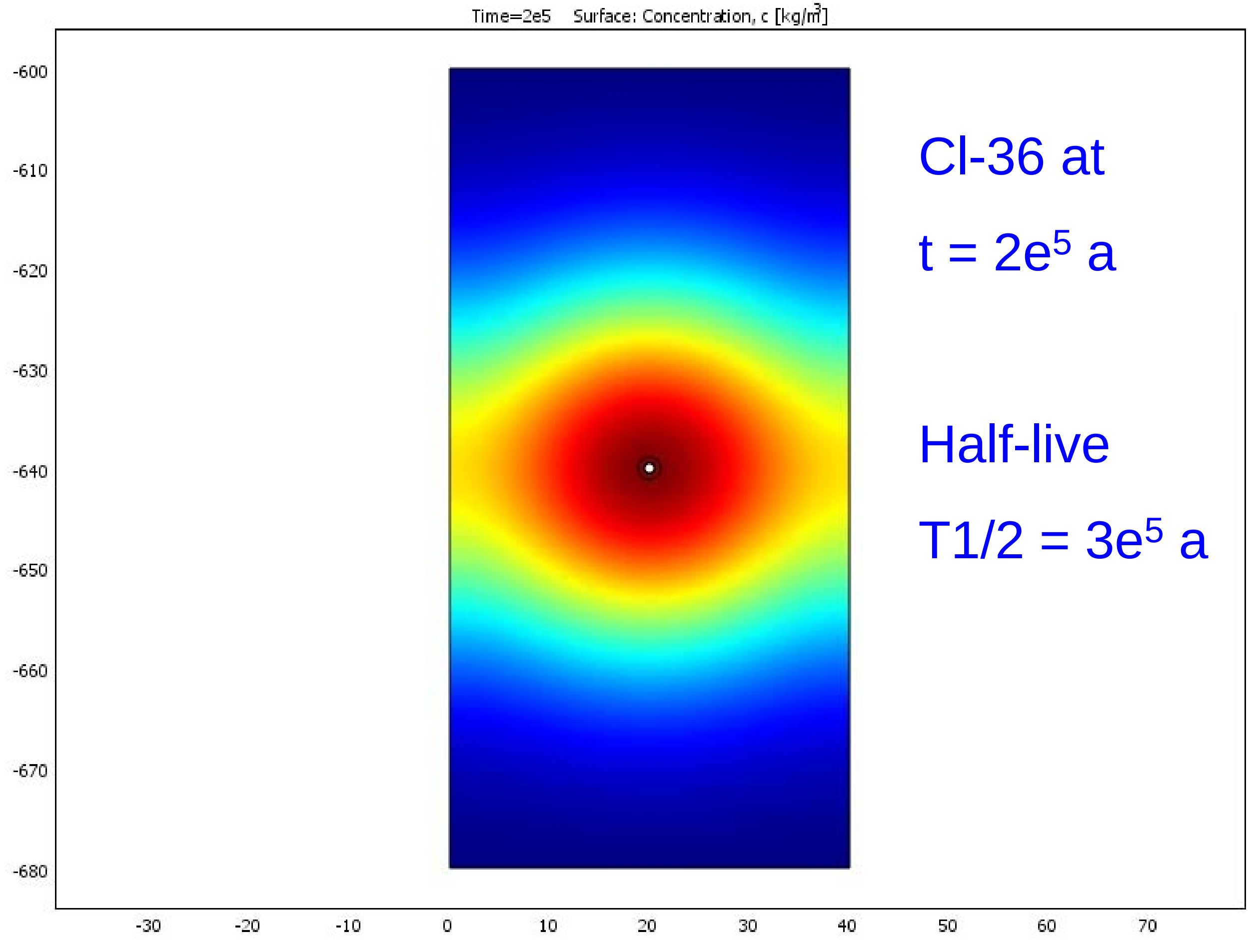


-600
-610
-620
-630
-640
-650
-660
-670
-680
-40
-30
-20
-10
0
10
20
30
40
50
60
70
80

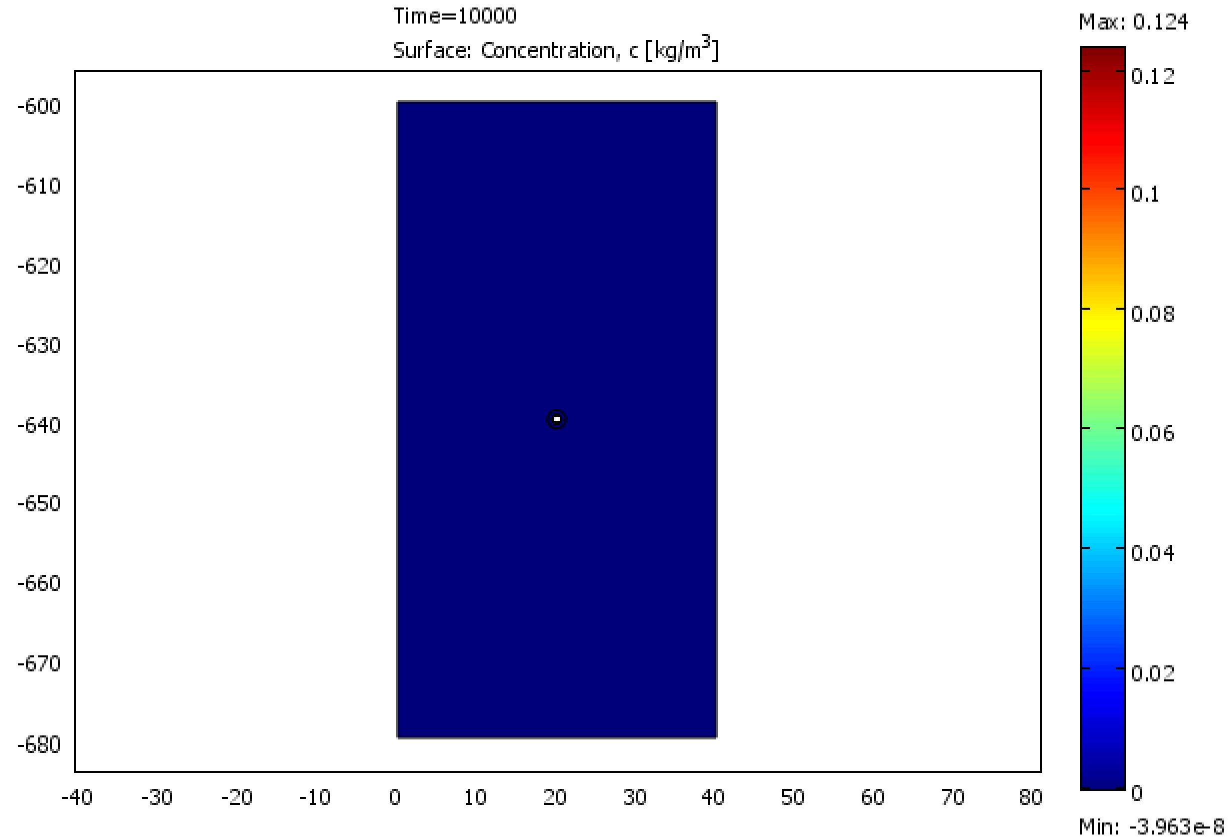
Stationary Flow Field



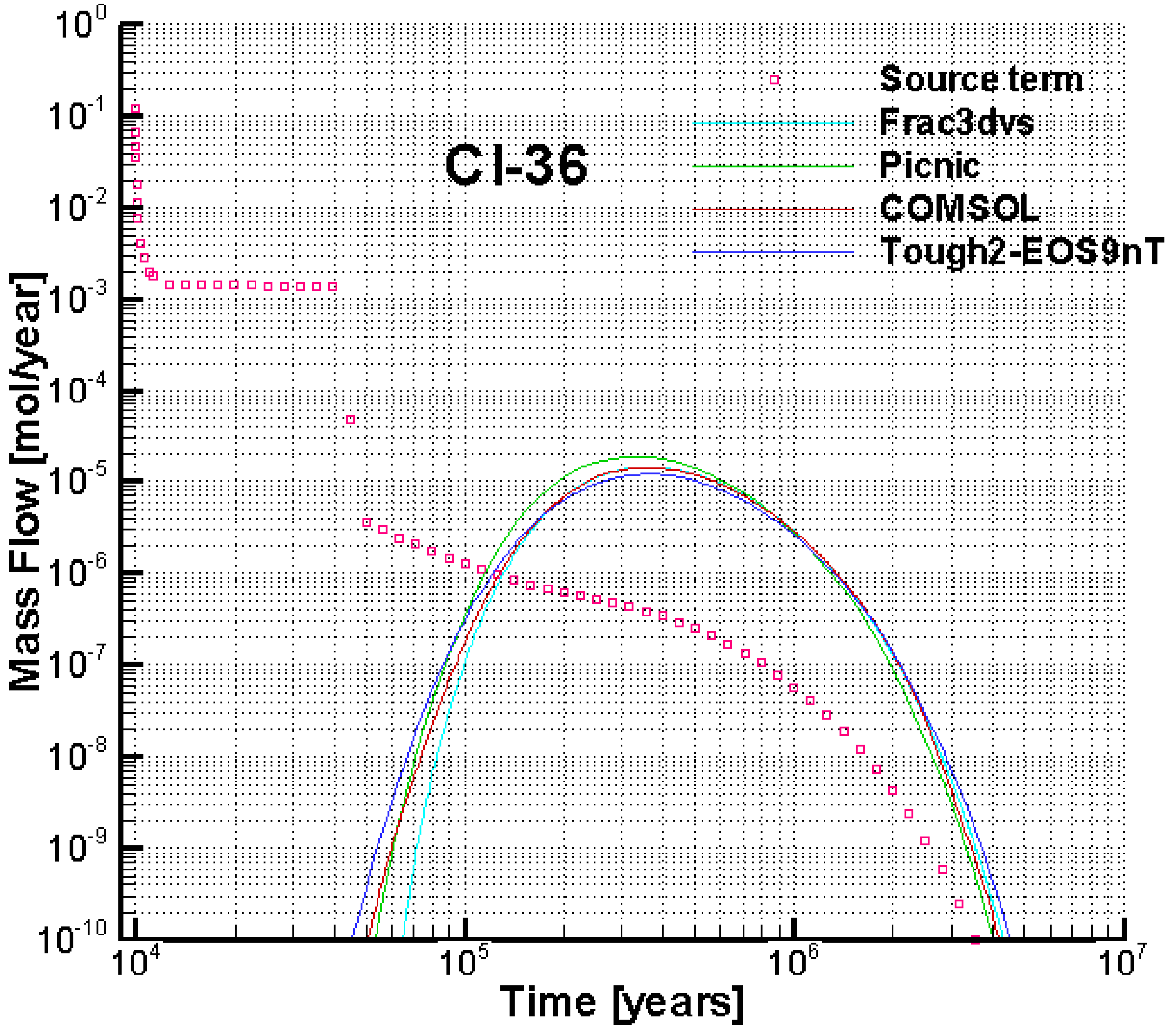
Concentration



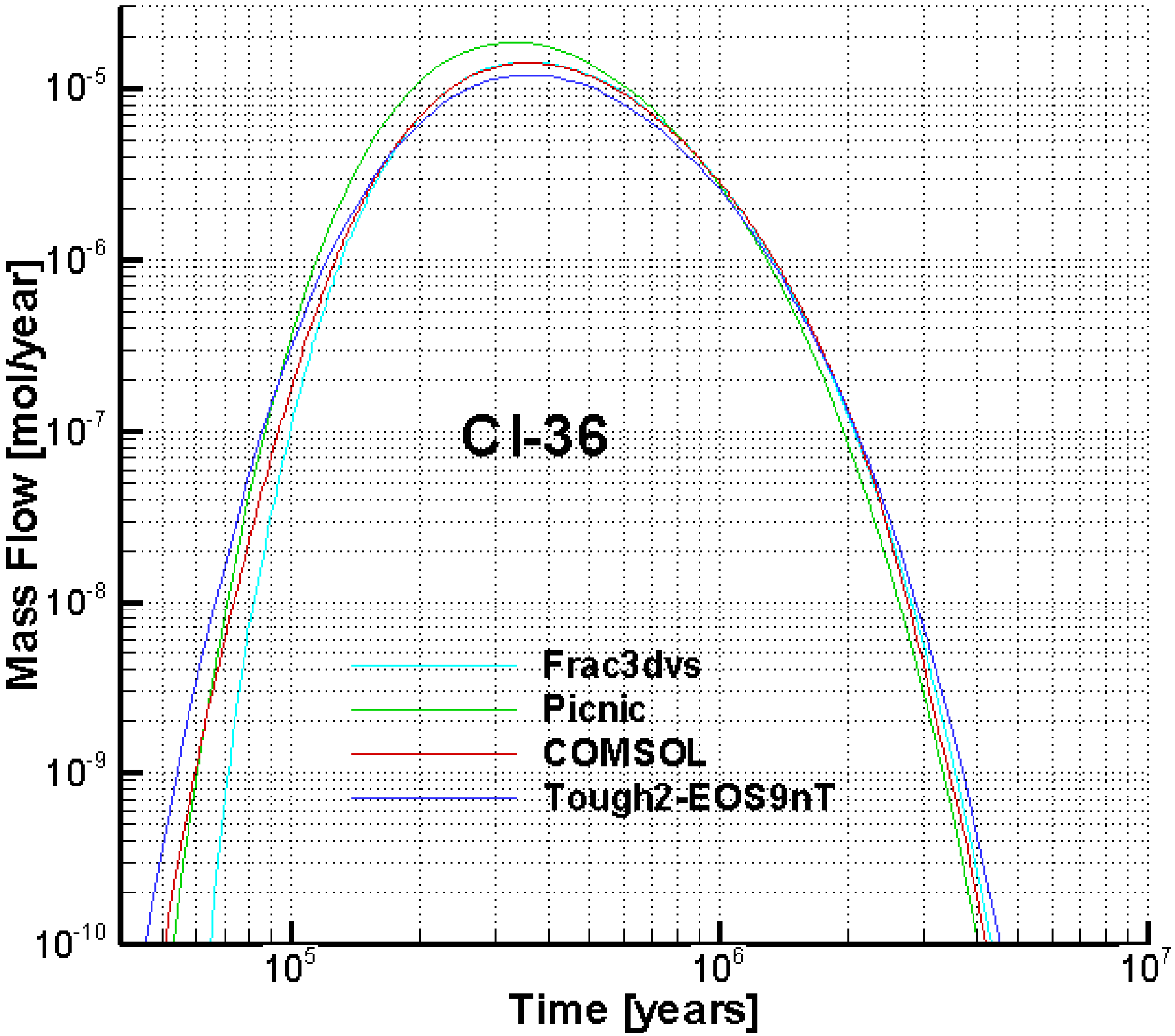
Concentration



Results, Release Rates for Cl-36



Results, Release Rates for Cl-36



Peak Concentration

Nuclide	Frac3dvs		Picnic		Comsol		Tough2-EOS9nT	
	Max. [mol/a]	$t_{max.}$ **[a]**	**Max. [mol/a]**	$t_{max.}$ **[a]**	**Max. [mol/a]**	$t_{max.}$ **[a]**	**Max. [mol/a]**	$t_{max.}$ **[a]**
Ca-41	$2.6\cdot10^{-10}$	$6.3\cdot10^{9}$	$2.8\cdot10^{-10}$	$6.3\cdot10^{5}$	$2.8\cdot10^{-10}$	$6.2\cdot10^{5}$	$2.8\cdot10^{-10}$	$6.2\cdot10^{5}$
C_{org}-14	$4.5\cdot10^{-8}$	$4.5\cdot10^{4}$	$5.9\cdot10^{-8}$	$4.5\cdot10^{4}$	$4.2\cdot10^{-8}$	$4.6\cdot10^{4}$	$4.2\cdot10^{-8}$	$4.5\cdot10^{4}$
Se-79	$5.3\cdot10^{-7}$	$1.4\cdot10^{6}$	$6.3\cdot10^{-7}$	$1.3\cdot10^{6}$	$5.6\cdot10^{-7}$	$1.4\cdot10^{6}$	$4.8\cdot10^{-7}$	$1.4\cdot10^{6}$
Cl-36	$1.4\cdot10^{-5}$	$3.6\cdot10^{5}$	$1.9\cdot10^{-5}$	$3.2\cdot10^{5}$	$1.4\cdot10^{-5}$	$3.6\cdot10^{5}$	$1.2\cdot10^{-5}$	$3.6\cdot10^{5}$
I-129	$2.2\cdot10^{-4}$	$1.3\cdot10^{6}$	$2.3\cdot10^{-4}$	$1.3\cdot10^{6}$	$1.9\cdot10^{-4}$	$1.4\cdot10^{6}$	$1.5\cdot10^{-4}$	$1.4\cdot10^{6}$

Maximum difference = 15%

Conclusions

- The generally good agreement between the results of different codes for various radionuclides cross-verifies the modelling approach and tools
- Small differences between the results can be attributed to different numerical methods
- The release curves provided by Frac3dvs and COMSOL are mostly in between those of Tough2-EOS9nT and Picnic
- Picnic takes mostly the largest values of concentration on the top of the breakthrough curve, probably because of the one-dimensional approach
- Tough2-EOS9nT takes mostly the largest values of concentration at the beginning of the curve, probably because of the interpolation of the source term
- Tough2-EOS9nT and COMSOL will further be used by ENSI