The COUPLEX Models

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Introduction

Motivations

– Develop a meaningful benchmark to compare transport codes

– Increase awareness of waste simulation issues within research community

– Identify critical numerical issues

3 test cases

Couplex 1 : far field simulation, simple physics

Couplex 2 : near field simulation, more physics (glass dissolution, simplified chemistry)

Couplex 3 : coupled near field / far field, research topic

Even first case was harder than it looked

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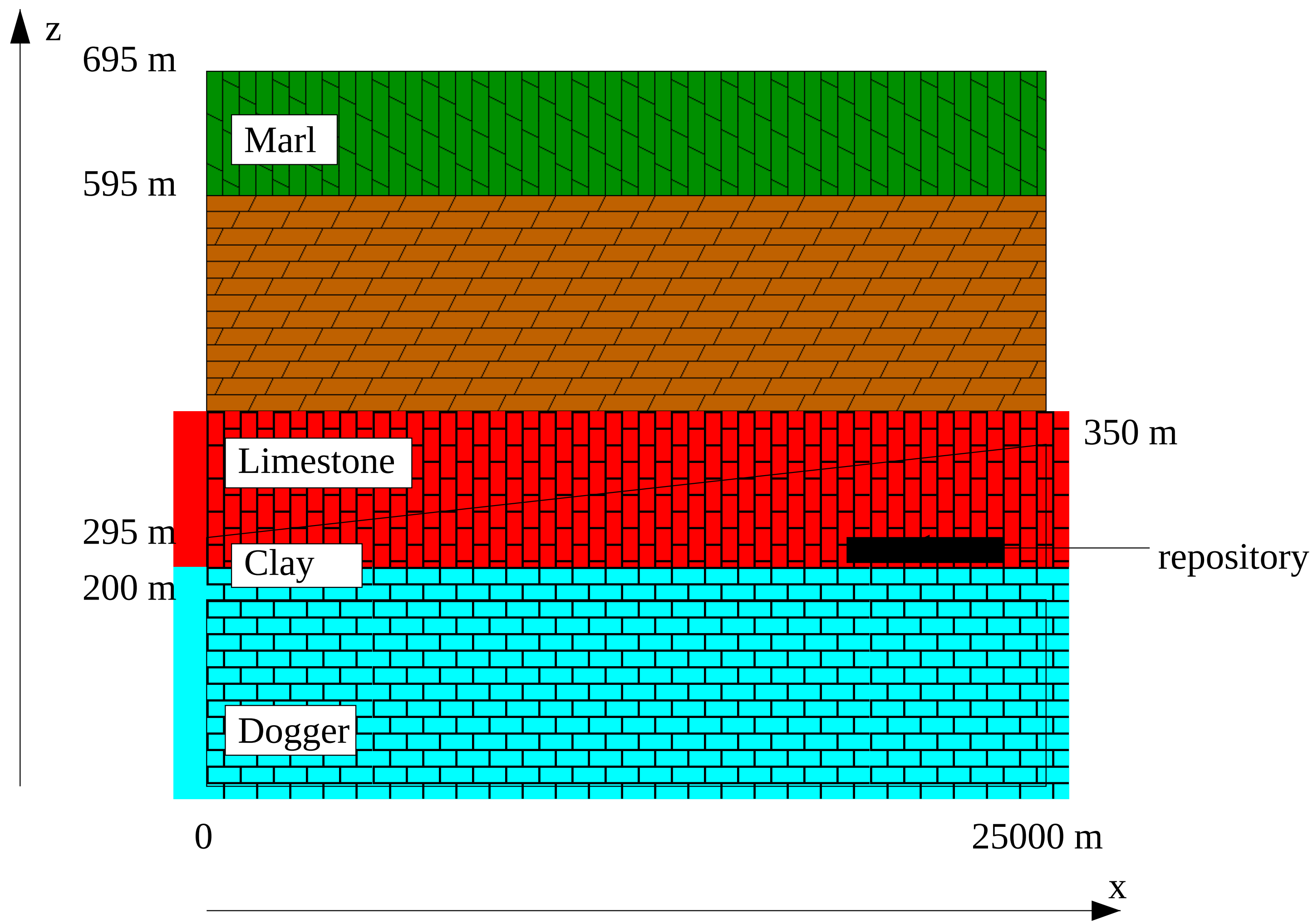
The COUPLEX 1 geometry



COUPLEX 1 physics – Flow

Darcy's law ($H = P/\rho g + z$ is piezometric head)

$$\mathbf{u} = -K \nabla H$$

Conservation of mass :

$$\nabla \cdot (K \nabla H) = 0 \quad \text{in } \mathcal{O}$$

Permeability constant in each layer

	Marl	Limestone	Clay	Dogger
K (m/year)	$3.1536\,10^{-5}$	6.3072	$3.1536\,10^{-6}$	25.2288

Boundary conditions :

- prescribed head
- no flow

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COUPLEX 1 physics – Transport

2 elements : Iodine 129 (half life : $1.6\,10^7$ years) , Plutonium 242 (half life : $3.8\,10^5$ years)

$$R_i\phi\frac{\partial C_i}{\partial t} + L(C_i) + R_i\phi\lambda_i C_i = f_i \quad \text{in } \mathcal{O}\times(0,T) \quad i = 1, 2.)$$

- R_i : Retardation factor
- ϕ : effective porosity
- $\lambda_i = \log 2/T_i$, T_i is half-life time of element

Transport operator : $\quad L(C) = -\nabla\cdot(\mathbf{D}\nabla C) + \mathbf{u}\cdot\nabla C$

$\mathbf{D}$ is diffusion/dispersion tensor :

$$\mathbf{D} = d_e I + |\mathbf{u}|\left[\alpha_l E(\mathbf{u}) + \alpha_t(I - E(\mathbf{u}))\right]$$

$$E_{kj}(\mathbf{u}) = \frac{u_k u_j}{|\mathbf{u}|^2}.$$

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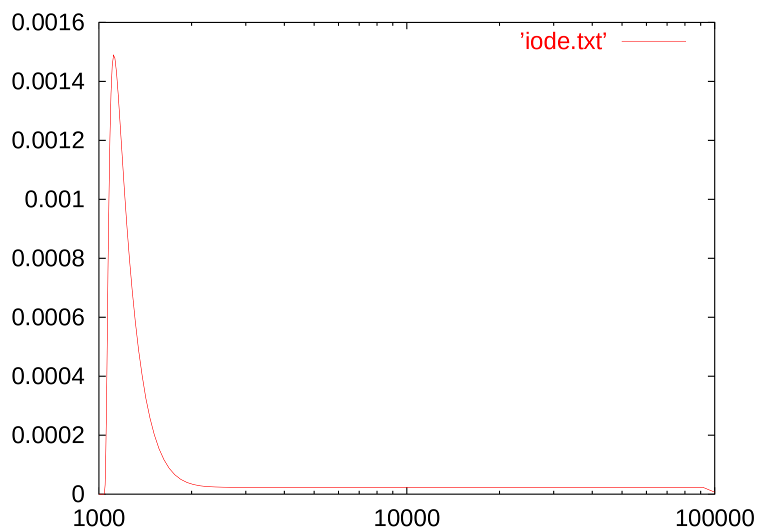
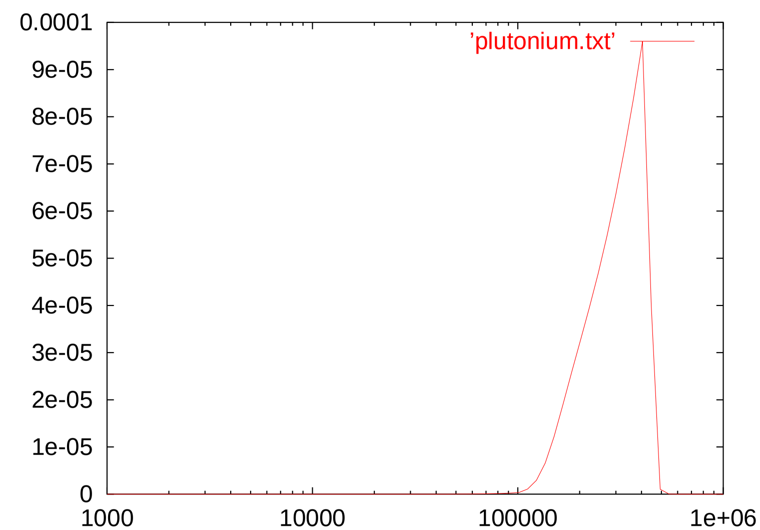
COUPLEX 1 physics – Sources

Concentrated in the repository, given as *known* time series





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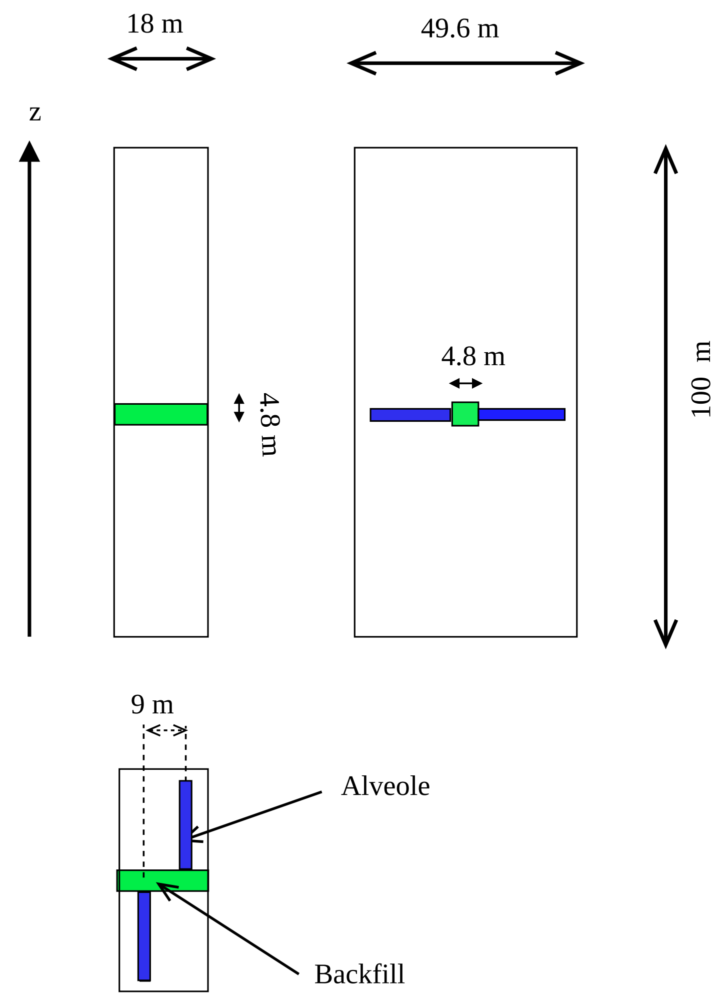
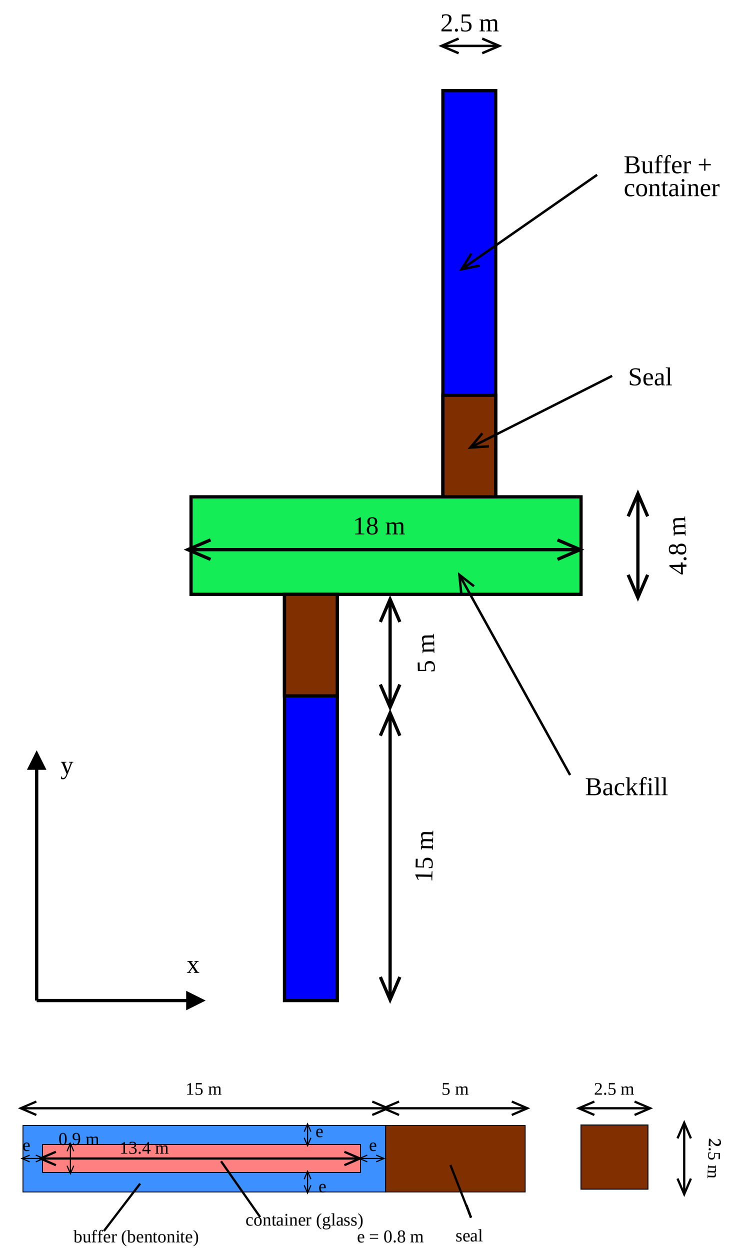
COUPLEX 2 geometry




2.5 m
Buffer +
container
Seal
18 m
4.8 m
5 m
Backfill
15 m
y
x
15 m
5 m
2.5 m
e
0.9 m
13.4 m
e
e
e
2.5 m
buffer (bentonite)
container (glass)
e = 0.8 m
seal

COUPLEX 2 physics – Overview

- Flow is again Darcy's law, with periodic BC on lateral boundaries, and known difference in head on top and bottom.
- Glass container dissolves over time. Nuclides are released in proportion to amount of dissolved silica.
- Transport of 1 isolated nuclide (Cesium 135), 2 chains (^{238}Pu $\rightarrow$ ^{234}U and ^{242}Pu $\rightarrow$ ^{238}U).
- Sorption modeled by isotherms, elementwise precipitation for Pu and U.

Have to solve for 10 coupled fields

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Transport equations

Silica $$\phi R_s \frac{\partial C_s}{\partial t} + L_s(C_s) = \rho_p \frac{\nu_p}{\lambda_p}\left(1 - \frac{C_s}{S_p}\right) \quad \text{in } R^* \backslash \bar{\mathcal{C}}$$

Cesium $$\phi \frac{\partial}{\partial t}(R_{\mathsf{Cs}} C_{\mathsf{Cs}}) + L_{\mathsf{Cs}}(C_{\mathsf{Cs}}) + \phi R_{\mathsf{Cs}} \lambda_{\mathsf{Cs}} C_{\mathsf{Cs}} = 0 \quad \text{in } R^* \backslash \bar{\mathcal{C}}$$

Plutonium $$\phi R_{\mathsf{Pu}} \frac{\partial C_{\mathsf{Pu}}}{\partial t} + L_{\mathsf{Pu}}(C_{\mathsf{Pu}}) + \phi R_{\mathsf{Pu}} \lambda_{\mathsf{Pu}} C_{\mathsf{Pu}} = \phi S_{\mathsf{Pu}} \quad \text{in } R^* \backslash \bar{\mathcal{C}}$$

Uranium $$\phi R_{\mathsf{U}} \frac{\partial C_{\mathsf{U}}}{\partial t} + L_{\mathsf{U}}(C_{\mathsf{U}}) + \phi R_{\mathsf{U}} \lambda_{\mathsf{U}} C_{\mathsf{U}} - \phi R_{\mathsf{U}} \lambda_{\mathsf{U}} C_{\mathsf{U}} = \phi S_{\mathsf{U}} \quad \text{in } R^* \backslash \bar{\mathcal{C}}$$

Plutonium and Uranium have solid phase (no transport), coupling between isotopes by precipitation.

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Boundary conditions

Provide release mechanism though glass dissolution.

Silica : First order dissolution on the glass-bentonite interface

$$-\mathbf{D}_s \frac{\partial C_s}{\partial n} = \rho_m \nu_m \left(1 - \frac{C_s}{S_m}\right), \qquad \text{on } \partial\mathcal{C}$$

Nuclides : Congruent release

$$\mathbf{D}_k \frac{\partial C_k}{\partial n} = \frac{N_k(t)}{N_s^0} \mathbf{D}_s \frac{\partial C_s}{\partial n}, \qquad \text{on } \partial\mathcal{C}$$

$N_k(t)$ are number of moles of the corresponding element at time t. Solution of a coupled set of differential equations expressing decay of element.

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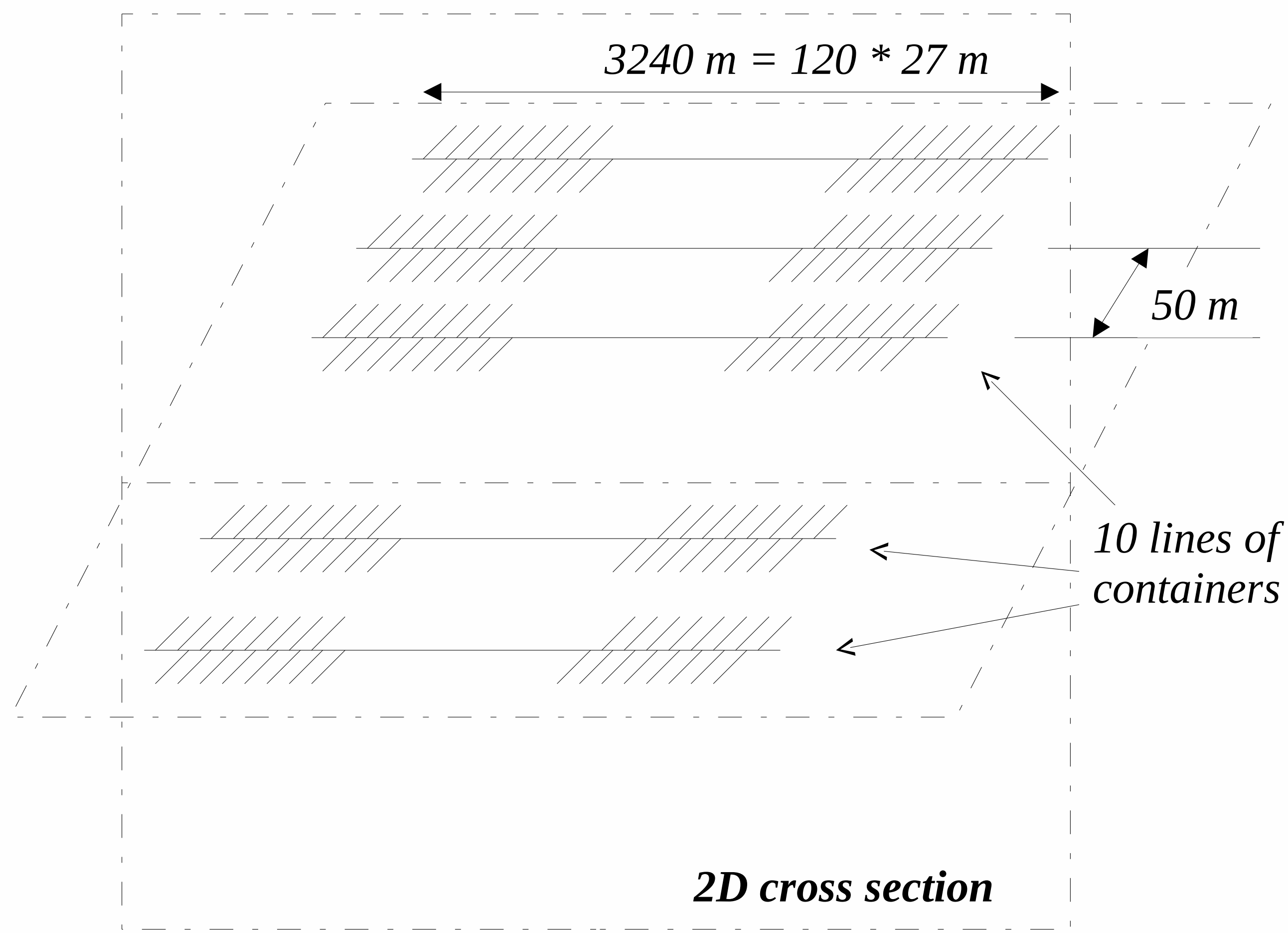
COUPLEX 3 geometry



Couplex 3

- Use results from Couplex 2 to obtain effective source term in Couplex 1
- Is there interaction between geoogic medium and repository ?
- Simplified repository : 10 lines of containers, each line with 120 times «Couplex 2» system.
- Can we do better than simple sum ?
- Coupling method not specified (actually not known).

This is a research problem

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