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STUDIECENTRUM VOOR KERNENERGIE
CENTRE D'ETUDE DE L'ENERGIE NUCLEAIRE

Building a Robust Numerical Model for Mass Transport Through Complex Porous Media

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ONDRAF/NIRAS

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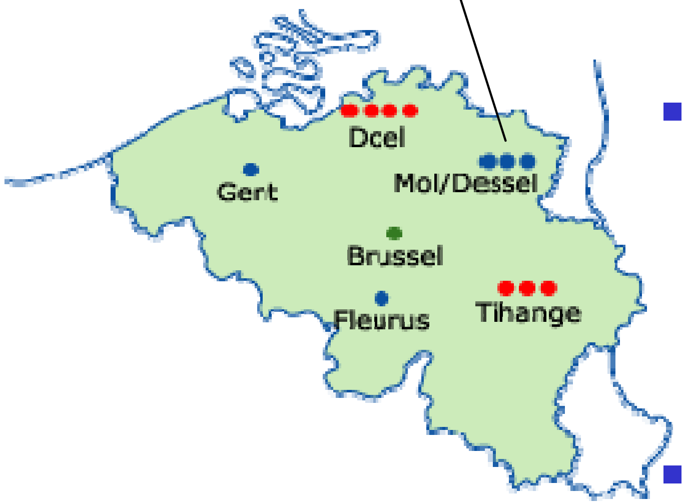
Background

Sources of radioactive waste in Belgium



- 7 nuclear power plants (5.5 GWe)
- Nuclear research (SCK•CEN, IRE, ...)
- Nuclear fuel fabrication plants (Belgonucleaire 1986-2006)
- The fabrication of radionuclides and their use in industry, medicine and research (Radium !)
- The dismantling of nuclear facilities (large volumes, relatively low activities)
- LILW-SL:
  - operational LILW-SL 18 700 m^3 (~75% NPP)
  - dismantling LILW-SL 51 800 m^3 (93% concrete)
- HLW: 2100 m^3 (reprocessing)

SCK•CEN
STUDIECENTRUM VOOR KERNENERGIE
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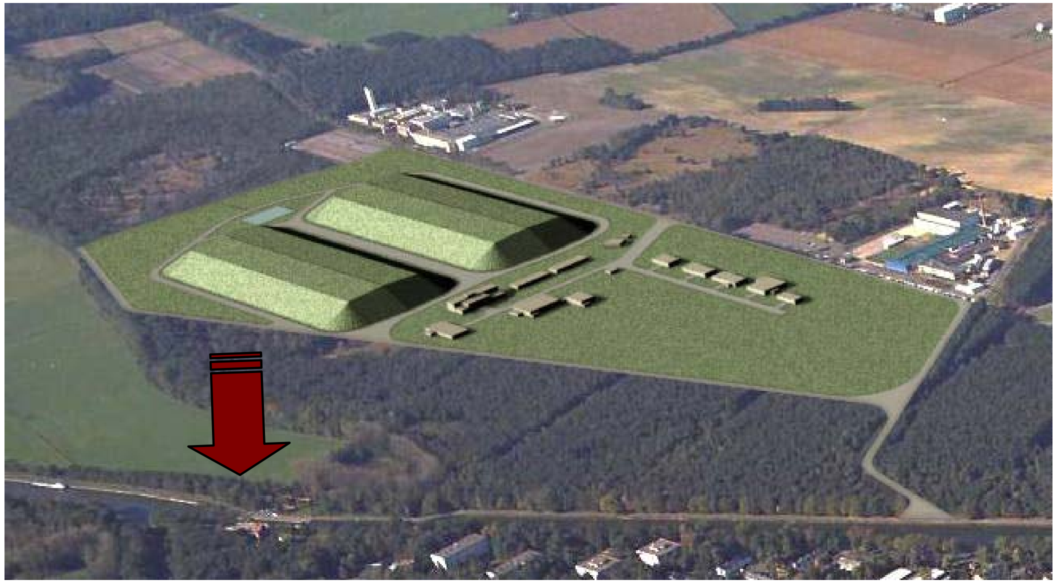
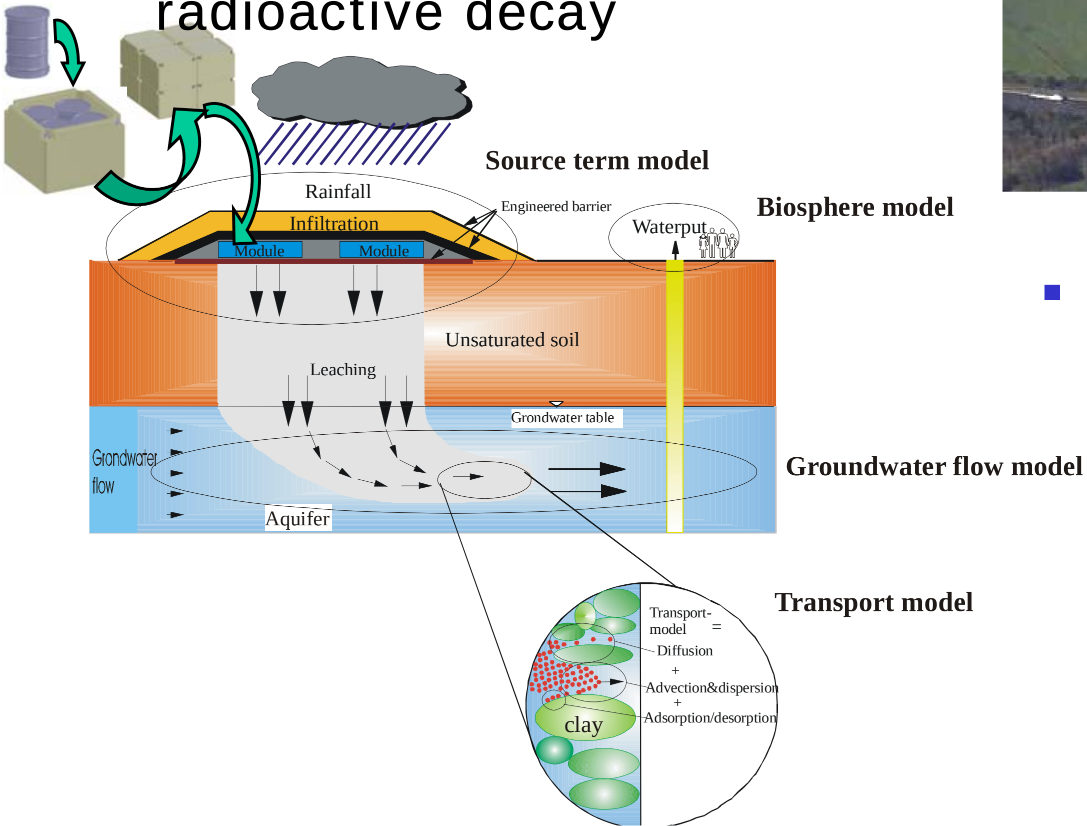
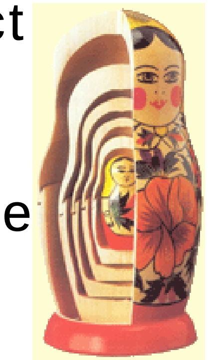
Background
General

- Long-term safety of surface disposal facility for radioactive waste (LILW-SL)
- The purpose is to isolate radionuclides from the environment >> allow for radioactive decay





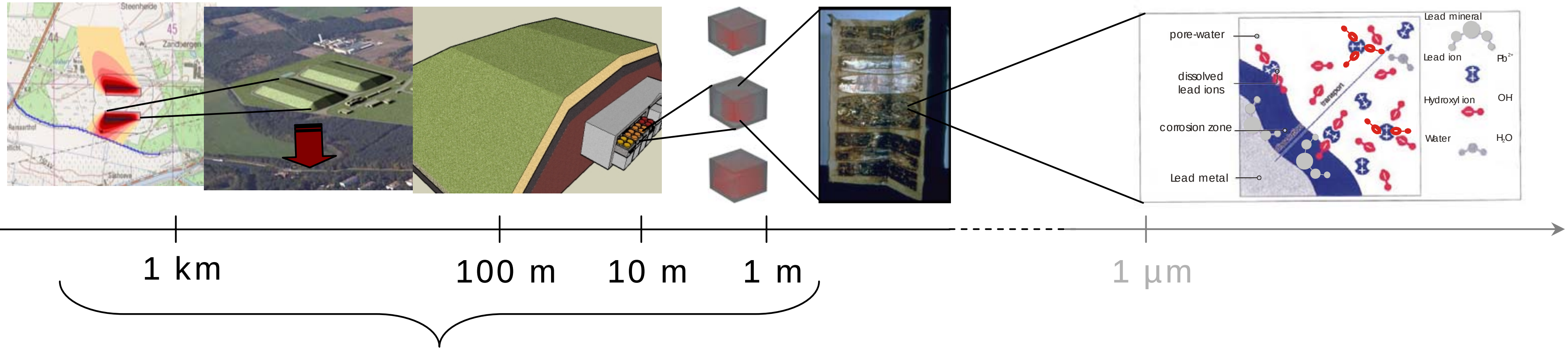
- Modelling radiological impact of radionuclide release from a multi-barrier repository to the geosphere and biosphere (i.e. humans) (Safety assessment)



Background

Some related issues

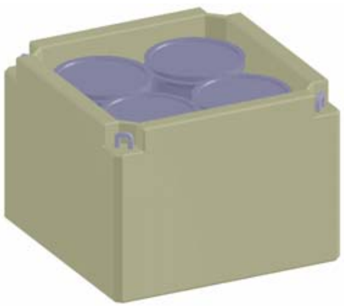
- Enormous **complexity** of interconnected physical-chemical phenomena acting on a wide range of length scales



- First simplification is division into three linear related components
  - Near field – transport of radionuclides through engineered barriers (**porous media**)
  - Geosphere – detailed modelling of groundwater flow and radionuclide migration
  - Biosphere – calculation of radiological impact from the use of groundwater for drinking, irrigation of fields and watering cattle

Background
Near field

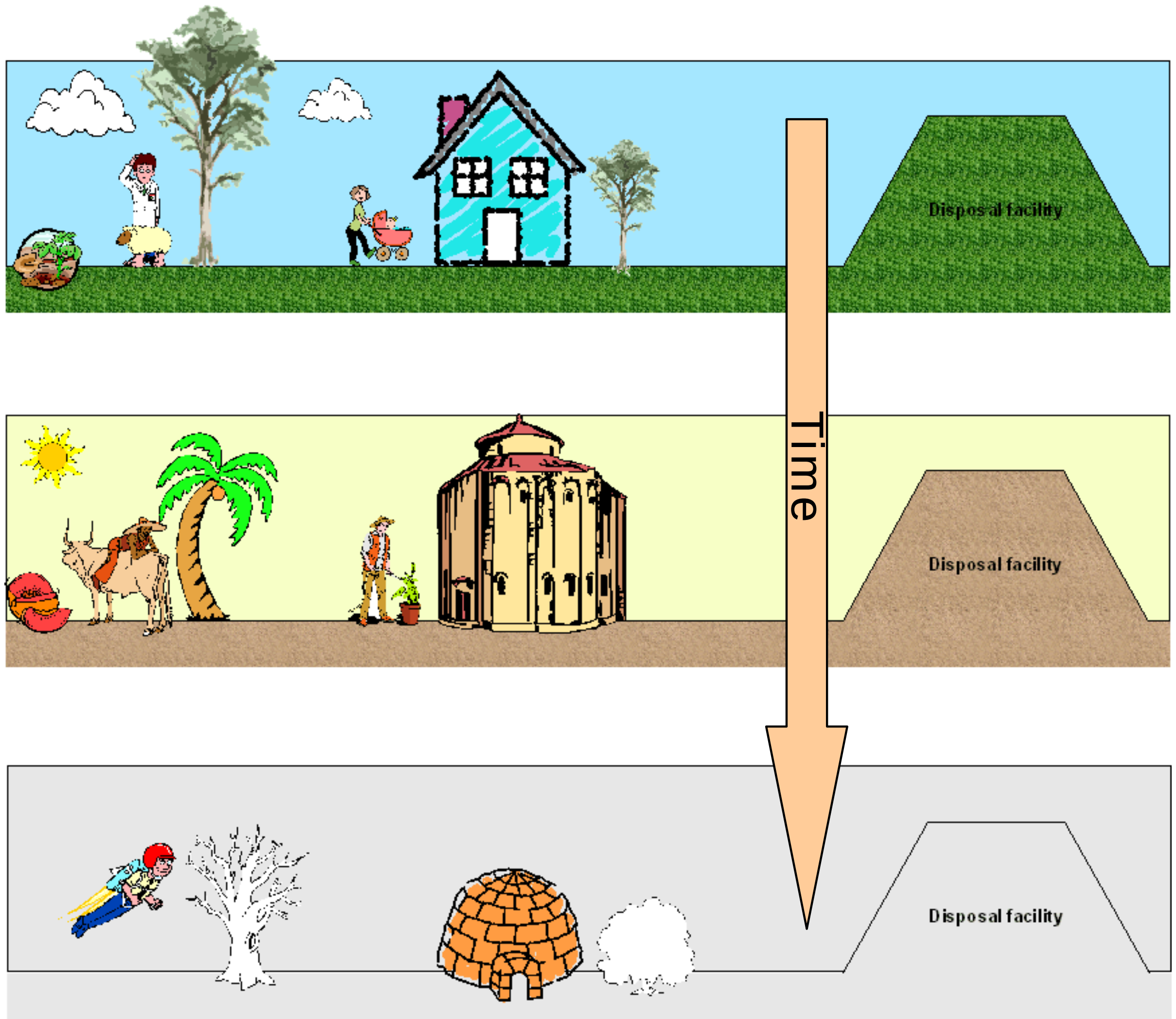
- Near field comprises
  - Multilayer cover (limit water infiltration)
  - Structural components of the vault (module) – e.g. concrete walls, floor, roof
  - Concrete waste disposal containers (monoliths)
    - ♣ Concrete “box” (different dimensions)
    - ♣ Conditioned waste (different dimensions and conditioning)+bulk waste
    - ♣ Backfill grout to fill void spaces between waste and box



Background
Time uncertainty

Time uncertainty

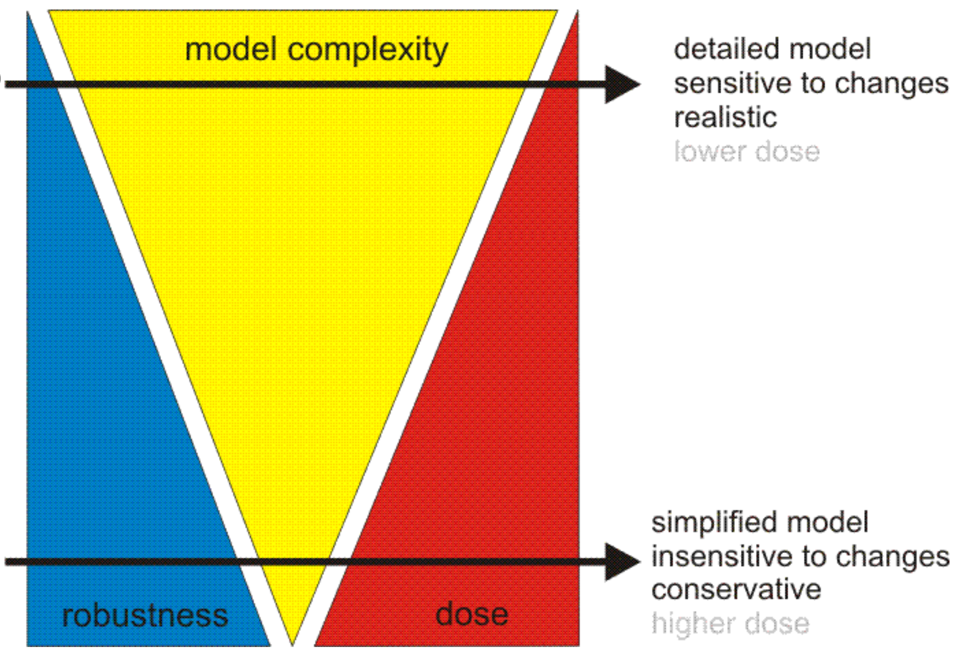
- Long time frames involved in modelling (10^6 y) which introduces uncertainty about:
  - Human habits
  - Physical parameters
  - Boundary conditions



Background
Conclusions

- Safety assessment over very long times can only provide qualitative results (order of magnitude estimates)
- Model simplification for dimensions, processes, boudary conditions required due to:
  - Large number of calculations
  - Too detailed models can be too sensitive
  - Lower dimension models are easier to explain
  - 3D models are numerically difficult to implement, time consuming and the least stable
  - Any simplification must be proven to be conservative

ROBUSTNESS



Radionuclide transport modelling
Numerical challenges

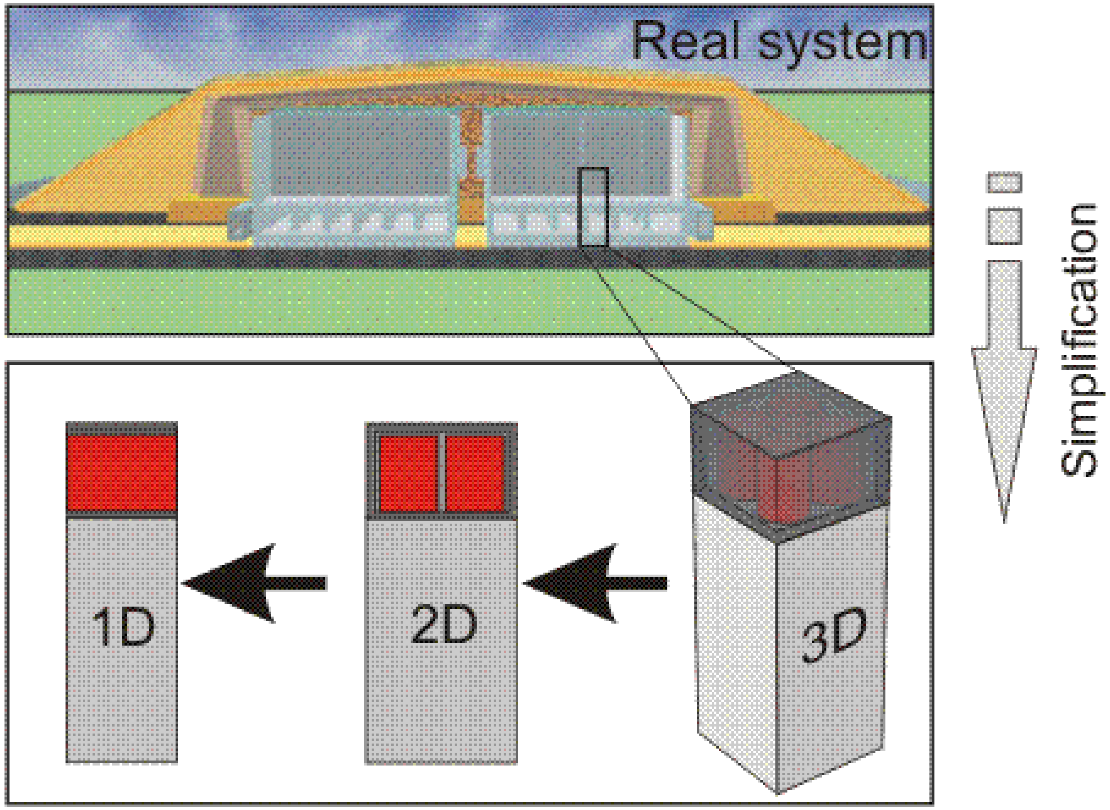
- Large difference between high initial concentrations in the source zone and low output concentrations (up to several tens of orders of magnitude)
  - Sensitive to numerical error (time and space discretization)
  - Any oscillation can lead to physically unrealistic result (negative concentrations)
- Oscillations may occur because of step function initial conditions, especially for high Pe numbers
- Solutions to avoid oscillations
  - Time and mesh discretization refinement at critical points
  - Smoothing of step functions (*flc2hs* COMSOL function)
  - Logarithmic concentrations ➡ seldom solves the problem
  - Streamline and/or crosswind diffusion

Easier implemented in 1D than in 3D!

Problem description

- The aim is to demonstrate the level of simplification still allowed for different contaminant release mechanisms
  - Instantaneous release
  - Diffusional release
  - Dissolutional release

Related to waste conditioning



- Use of COMSOL Multiphysics!

Physics and modelling approach
Instantaneous release

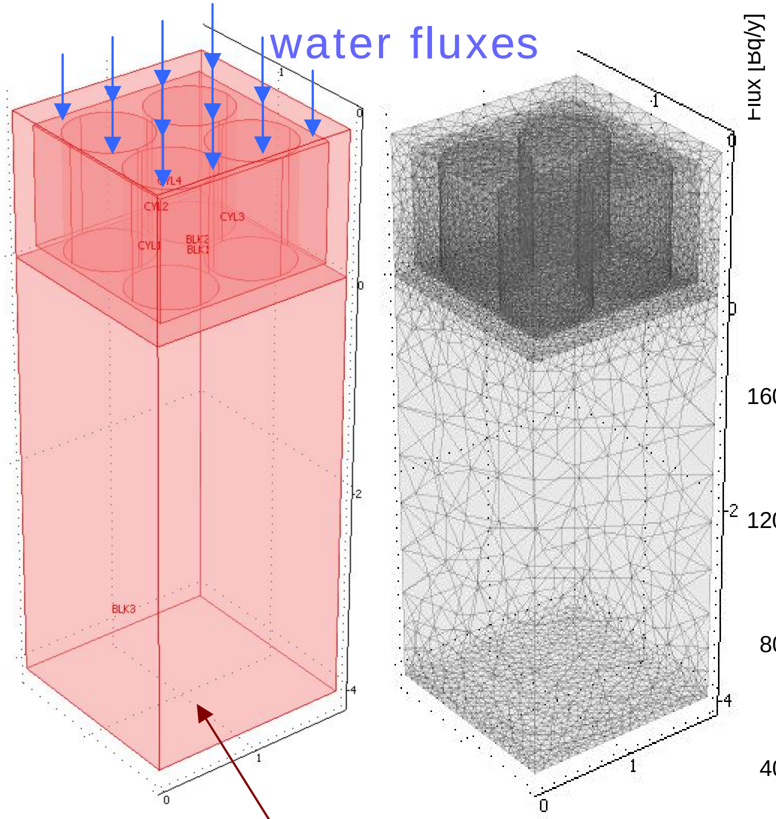
- Instantaneous release assumes all source activity is released instantaneously and completely
- This is the most conservative release model
- Radionuclides are leached from the conditioned waste by infiltrating water and by diffusion
- Imposed uniform water flux across the facility
  - Corresponds to degraded concrete (highly conservative)
  - Concrete retains sorption properties for contaminants
  - Simplifies the migration problem to solute transport equation only
- Comparison of leaching rates in 3D, 2D and 1D for two drum types (220 ***l*** and 400 ***l***) and two radionuclides (^{36}Cl and ^{129}I)

Physics and modelling approach

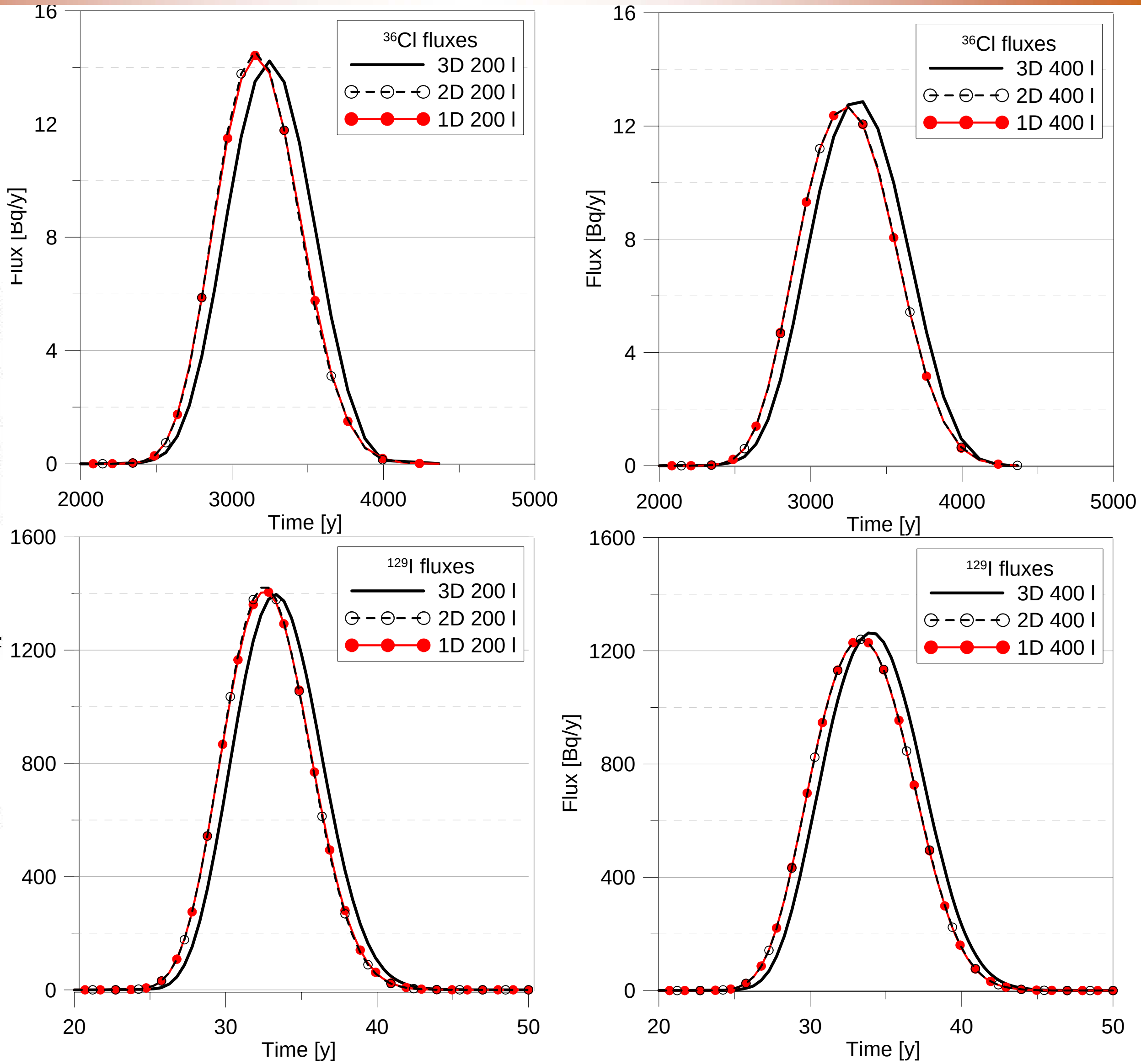
Instantaneous release

3D model example

Geometry Mesh

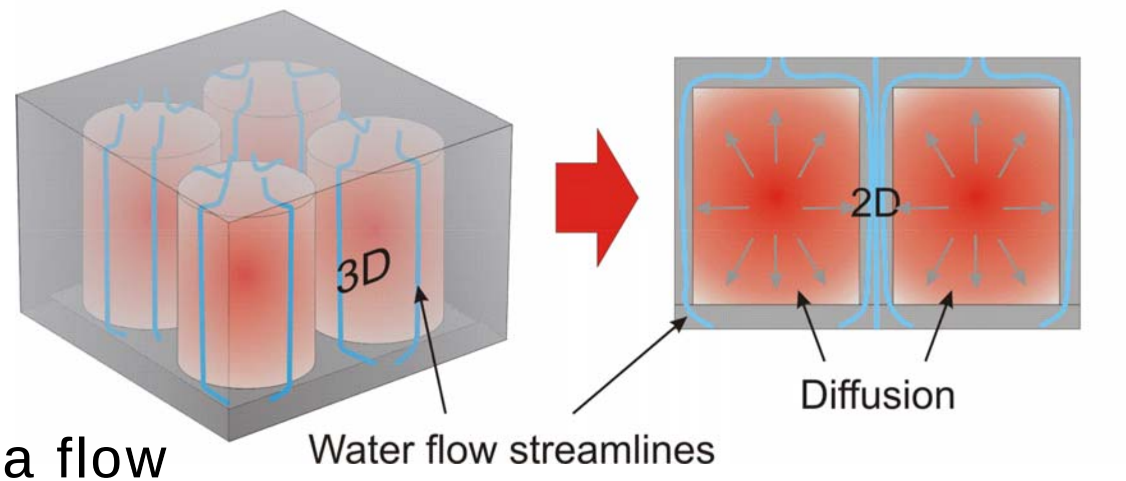


Integrated radionuclide fluxes



Physics and modelling approach
Diffusional release

- Diffusional release is the release of radionuclides by diffusion through a porous waste form only
  - e.g. cement-conditioned waste form or bituminized waste
- Water flow through the waste form is considered negligible
  - Water flow flows around the waste form



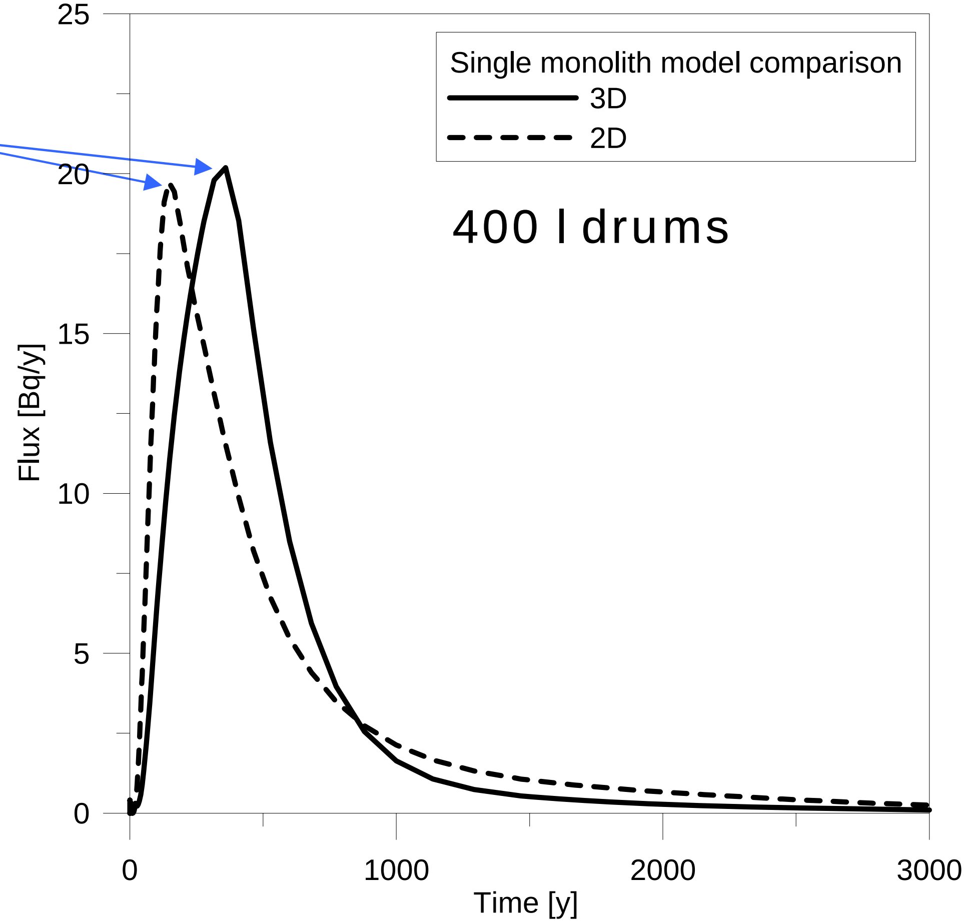
- Decoupled calculation
  - Saturated porous media flow
  - Solute transport (diffusion in waste form, advection outside)

Physics and modelling approach
Diffusional release

- Good agreement between 3D and 2D (implementation in 1D is not appropriate)
- Comparison should be made for each packaging type separately

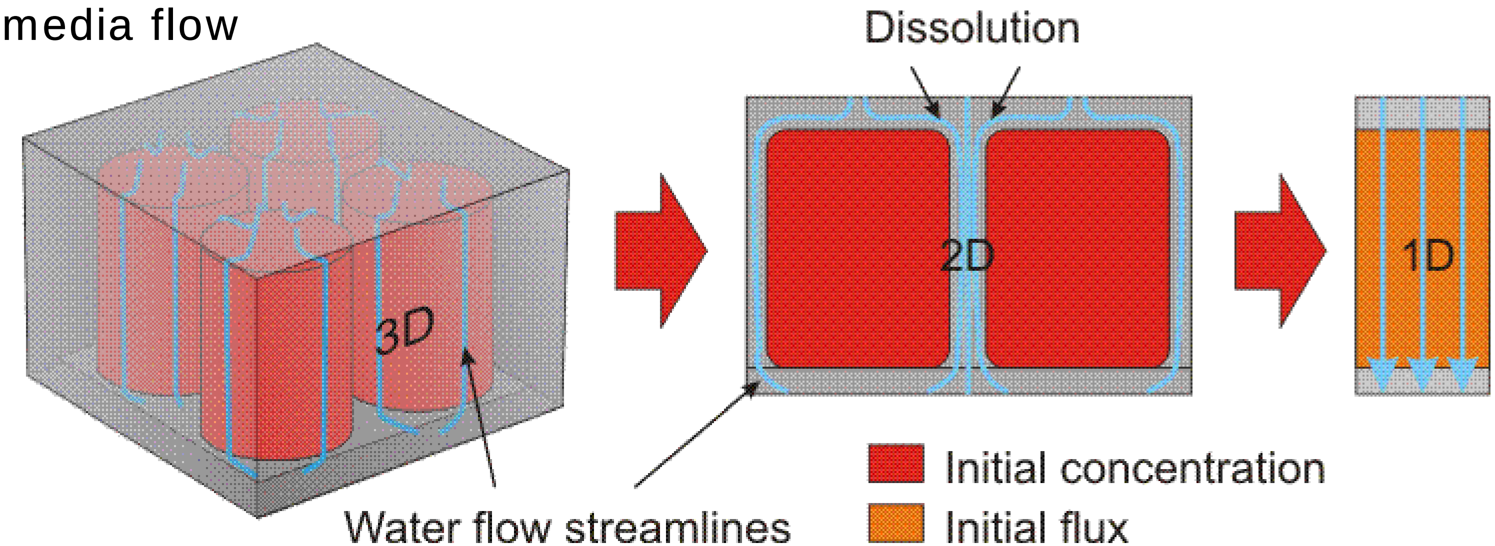
Peak fluxes in good agreement

Shift in time due to smoothing of source term



Physics and modelling approach
Dissolutional release

- Mass release is controlled by the time-dependent dissolution of the waste form
  - e.g. dissolution of vitrified waste, corrosion of steel
- Dissolutional release propagates from the waste form surface inward
- Different source term modeling approach in different dimensions
  - Applied initial concentration in 3D/2D
  - Applied flux in 1D
- Coupled calculation
  - Saturated porous media flow
  - Solute transport



Physics and modelling approach

Dissolutional release

- Dissolution defined by dissolution rate δ [m/y]
- Due to dissolution, radius r(t) and height z(t) of the source and consequently also reactive surface area A(t) decrease

$$r(t) = \begin{cases} r_0 - \delta t & r_0 \geq \delta \cdot t \\ 0 & r_0 < \delta \cdot t \end{cases} \qquad z(t) = \begin{cases} z_0 - \delta t & z_0 \geq \delta \cdot t \\ 0 & z_0 < \delta \cdot t \end{cases} \qquad A(t) = 2 \cdot \pi \cdot r(t)\left(r(t) + z(t)\right)$$

- Smoothed change of hydraulic conductivity

$$e^{\ln k_0 (1 - smooth(t)) + \ln k_1 \cdot smooth(t)}$$

$$smooth_z = flc2hs(z(t) - z_{bot}, 0.03) + (1 - flc2hs(z(t) - z_{top}, 0.03)) - 1$$

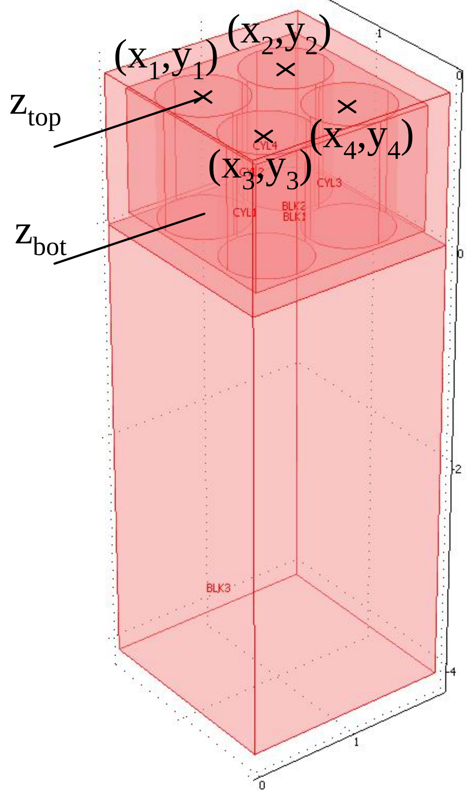
$$smooth_1 = 1 - flc2hs(\sqrt{(x(t) - x_1)^2 + (y(t) - y_1)^2}) - r, 0.03)$$

$$smooth_2 = 1 - flc2hs(\sqrt{(x(t) - x_2)^2 + (y(t) - y_2)^2}) - r, 0.03)$$

$$smooth_3 = 1 - flc2hs(\sqrt{(x(t) - x_3)^2 + (y(t) - y_3)^2}) - r, 0.03)$$

$$smooth_4 = 1 - flc2hs(\sqrt{(x - x_4)^2 + (y - y_4)^2}) - r, 0.03)$$

$$smooth(t) = smooth_z \cdot (smooth_1 + smooth_2 + smooth_3 + smooth_4)$$

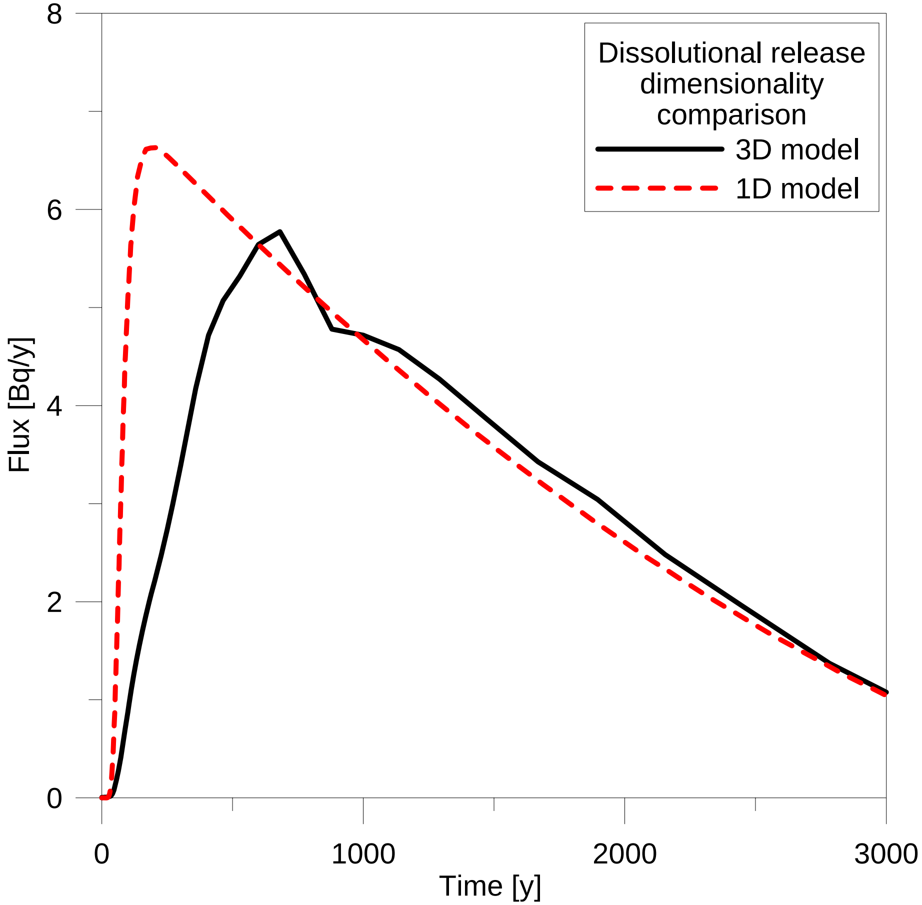


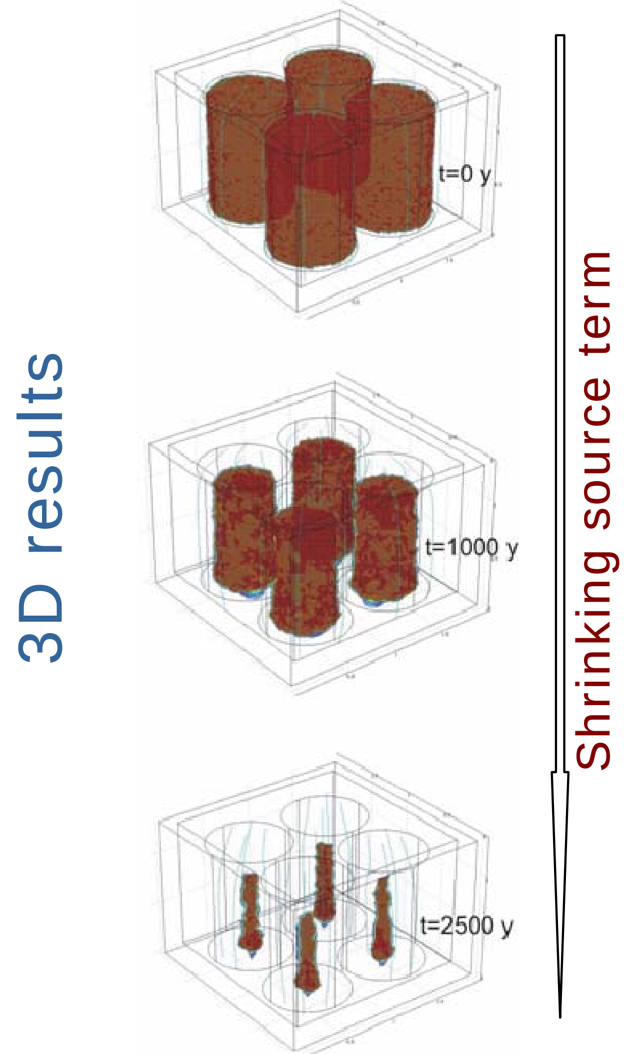
Physics and modelling approach
Dissolutional release

- In 1D the source is defined as radioactive flux

$$F_C[Bq/y] = C_0 \cdot \delta \cdot A(t) \cdot e^{-\ln(2)/T_{1/2} \cdot t}$$

$$T_{1/2} \text{....half life}$$



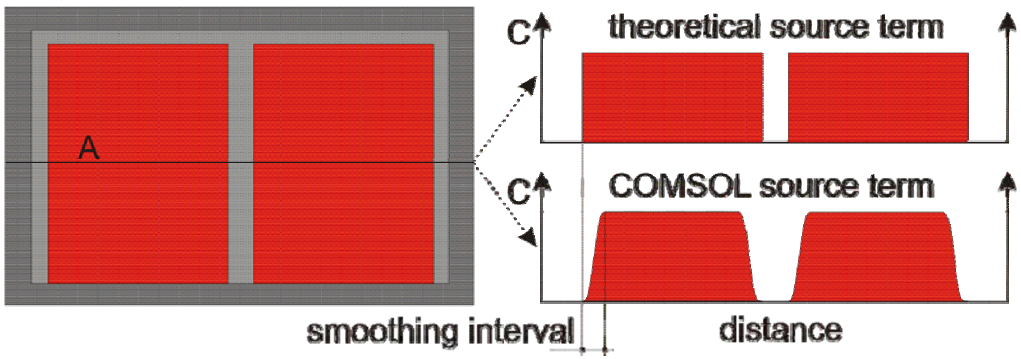


Conclusions

- Dimensionality reduction should be verified for each different conceptual model
- Sometimes simplification to 1D is not possible (diffusional release)
- For dissolutional release 3D calculations are time consuming
  - less than minute for 1D and 19 hours for 3D calculation
- Instantaneous release model (as defined here) gives equal results in 1D and in 3D
- COMSOL Multiphysics proved to be efficient and versatile tool for safety assessment calculations

Physics and modelling approach
Source term

- The problem involves solute transport of decaying and sorbing substances (i.e. radionuclides) in saturated porous media
- Initial condition: concentration in porewater $C(t_0) = \frac{A}{V \cdot R \cdot \eta}$
- Smoothing applied



- Volume correction due to smoothing $V = \int_V smooth \, \mathrm{d}V$
- Concentration with smoothing $C(\vec{x}, t_0) = smooth \cdot C(t_0)$