COMSOL CONFERENCE 2018 BOSTON

iWATER — Innovative Water Technologies for Environmental Research

YORK UNIVERSITÉ UNIVERSITY

nwmo — NUCLEAR WASTE MANAGEMENT ORGANIZATION / SOCIÉTÉ DE GESTION DES DÉCHETS NUCLÉAIRES

Diffusive Transport in a Deep Geological Repository for Used Nuclear Fuel

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NWMO: Who We Are

- Formed in 2002 as required by *Nuclear Fuel Waste Act*
- Funded by Canada's nuclear energy corporations
- Operates on a not-for-profit basis

Our mission is to develop and implement collaboratively with Canadians, a management approach for the long-term care of Canada's used nuclear fuel that is socially acceptable, technically sound, environmentally responsible, and economically feasible.

Site Selection Process: Initiated May 2010

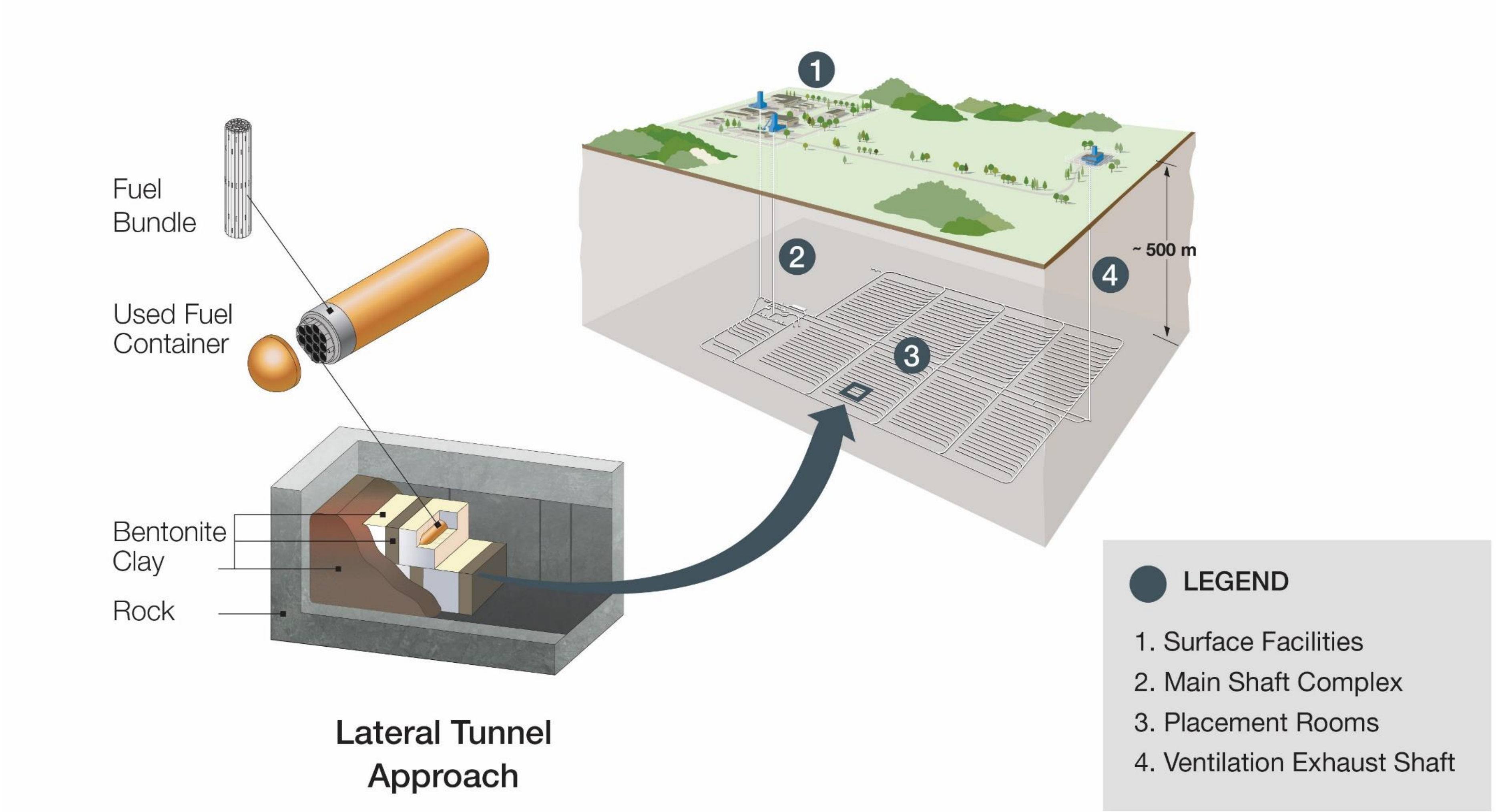
Seeking an informed and willing host with a suitable geologic formation:

- Multi-stage technical and socio-economic assessment approach
- Phased process over many years
- Communities expressed interest to participate
- Communities can choose to leave the process

Centralized containment and isolation of used nuclear fuel in a deep geological repository

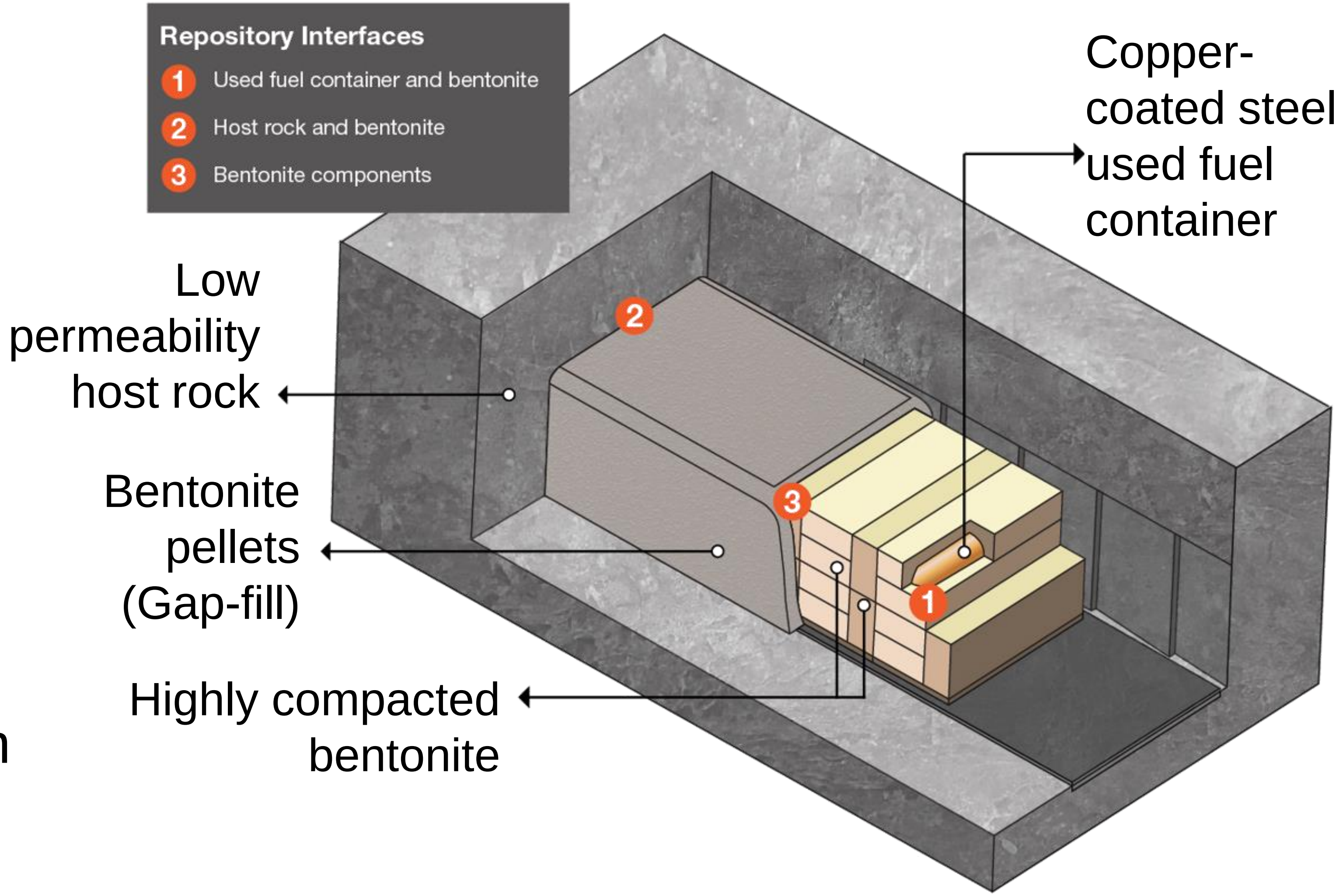
The project will only proceed with interested community, First Nation and Métis communities and surrounding municipalities working in partnership.

Deep Geological Repository (DGR)



Natural and Engineered Barriers in a DGR

- Multiple barriers between used fuel and the environment including:
  – Host rock
  – Bentonite
  – UFC (copper coated)
- Copper is a naturally stable metal but can be susceptible to sulphide corrosion
- Sulphate reducing bacteria in the host rock could produce sulphide.



Sulphide Transport Modelling

- Steady state, isothermal analysis
- Transient, thermal analysis (1 million years)
- Sensitivity analysis of:
  - Concentration gradient
  - Diffusion coefficient
  - Buffer box size (bentonite thickness)
  - Preferential pathways (hot spots, fractures, bentonite failure)

- The model was developed to aid in the safety assessment of the copper coating

Methods and Assumptions

Sulphide Production:

$$2Cu(s) + HS^{-} + H^{+} \rightleftarrows Cu_2S(s) + H_2$$

Fick's Law of Diffusion:

$$J = -D\nabla C$$

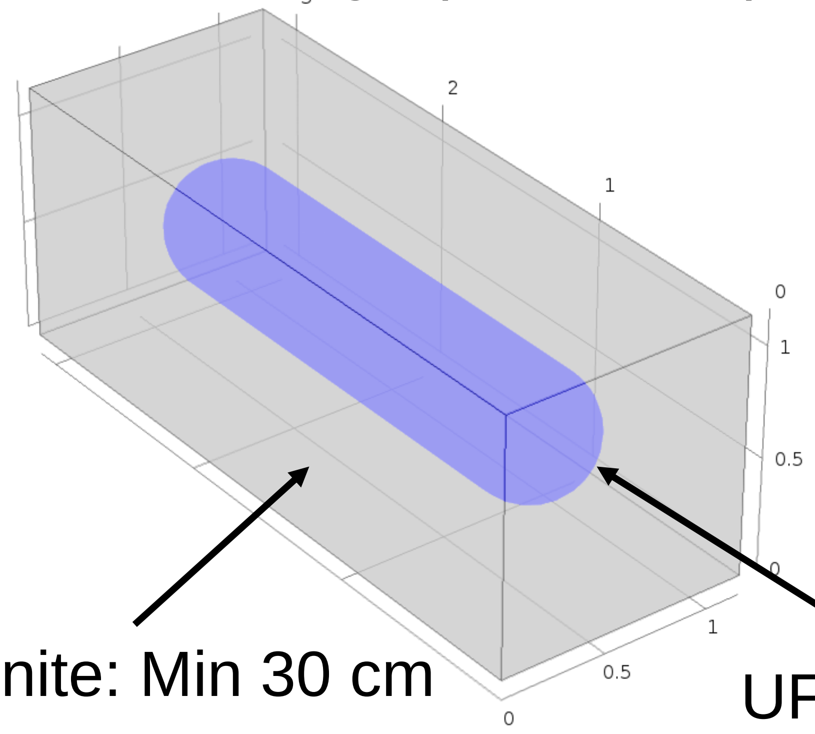
Corrosion Depth:

$$d_{corr} = \frac{N_{HS} f_{HS} M_{cu}}{A_{corr} \rho_{cu}}$$

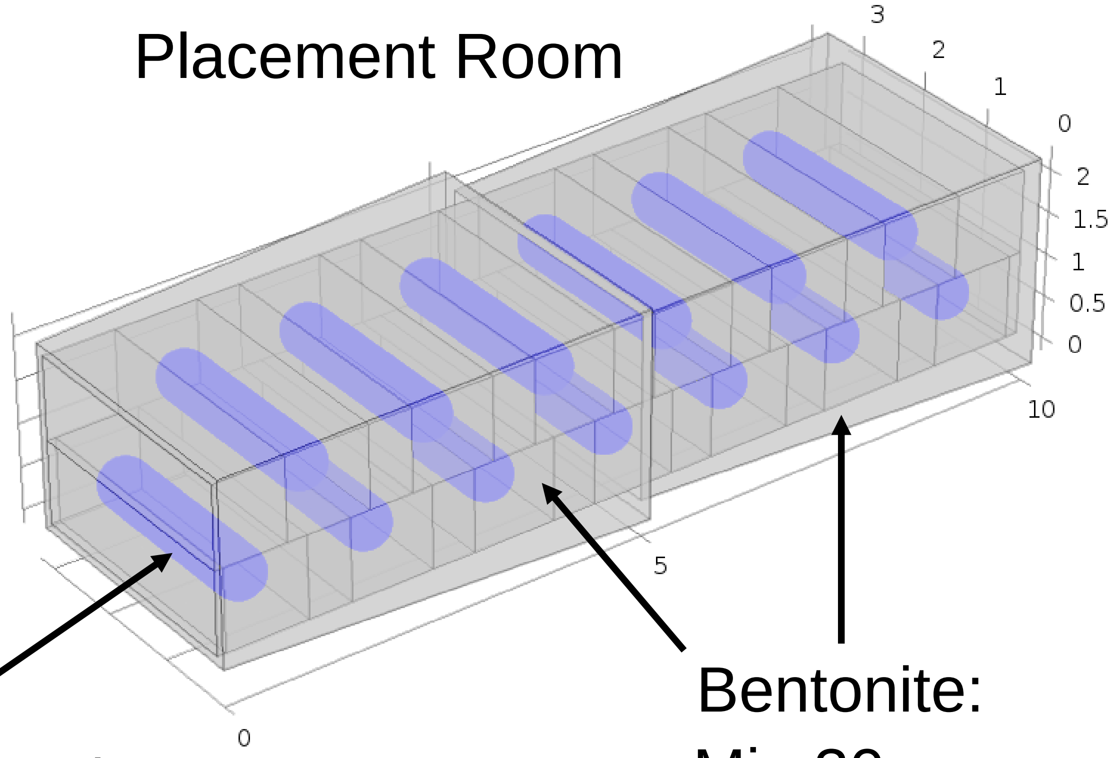
It is assumed that diffusion is the only process taking place (no active SRB, geochemistry, advective flux …) in a homogenous bentonite.

Model Geometry and Boundary Conditions

UFC Package (Buffer Box)



Placement Room



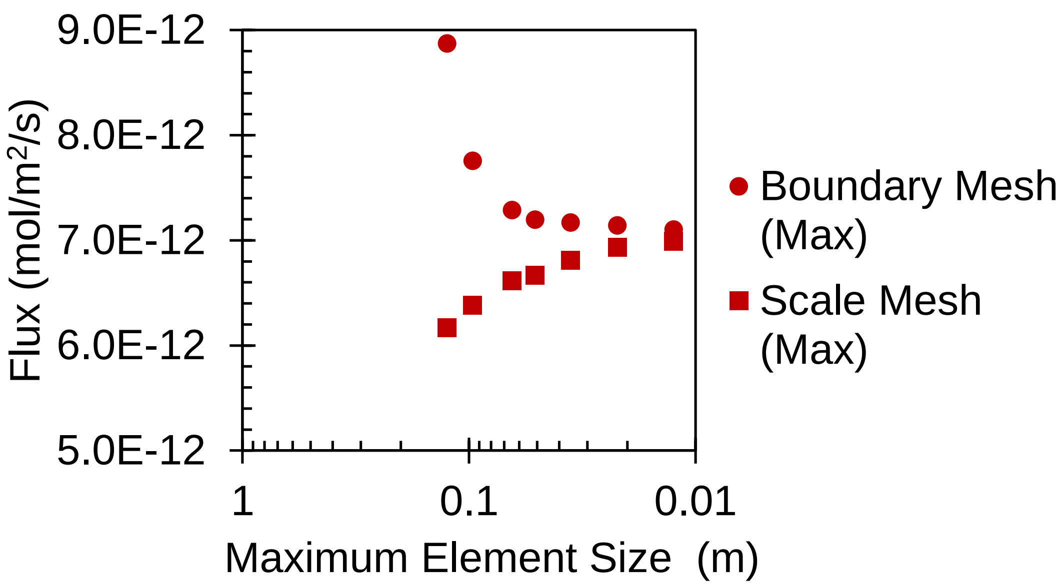
Bentonite: Min 30 cm

UFC (Zero Conc.)

Bentonite:
Min 30 cm

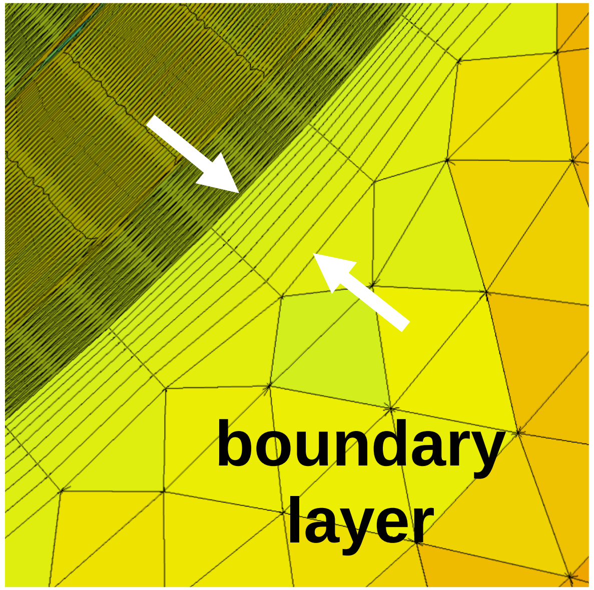
Constant sulphide concentration surrounding each model geometry

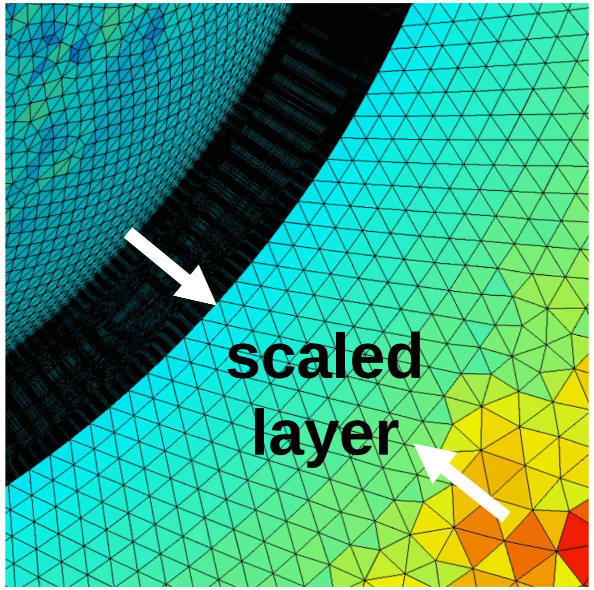
Model Implementation



Mesh Development:

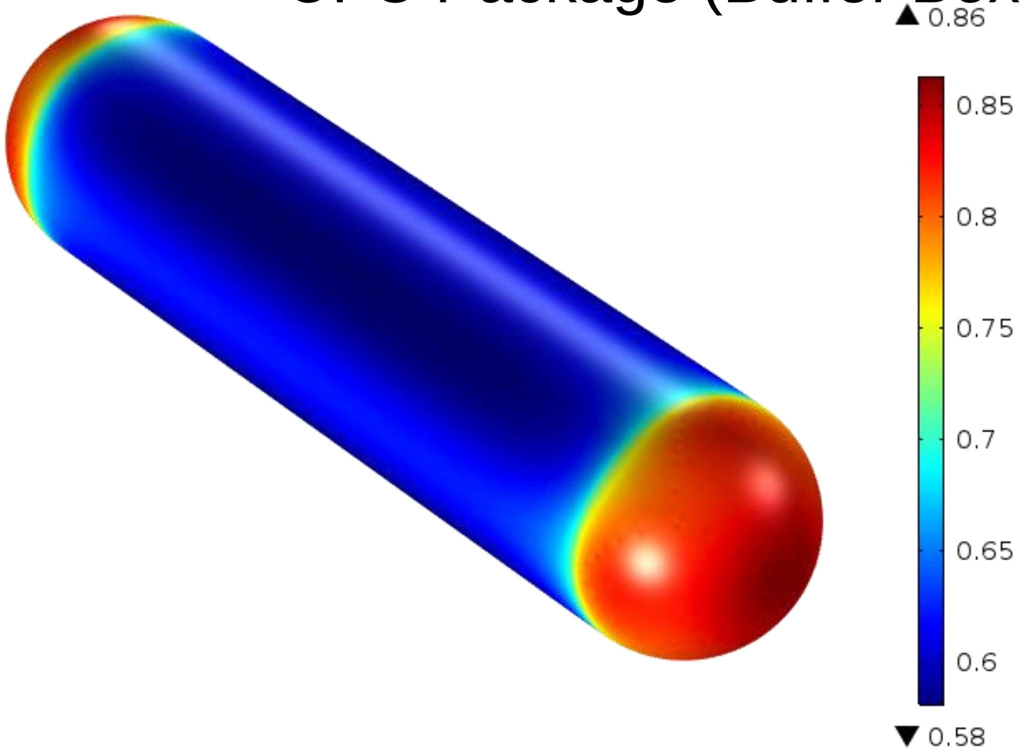
- Compared two mesh types
- Ensured a mesh size independent solution.
- Single UFC: 18.7 million elements (max: 0.015m)
- Placement Room: 20.6 million elements (max: 0.03m)
- Time dependent solve time ~ 1 day



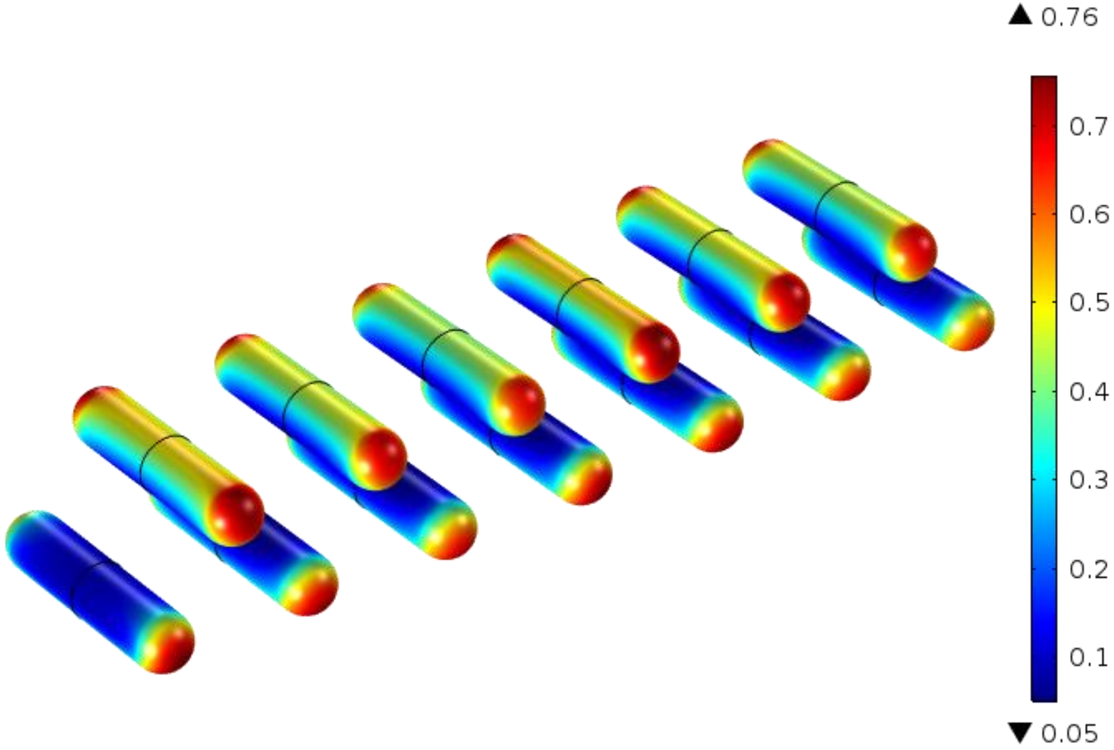


Steady State Sulphide Transport

UFC Package (Buffer Box)



Placement Room



MIC rate nm/year/PPM sulphide

Sulphide flux reaching the surface of a UFC placement room with minimum 30 cm bentonite. Highest flux values occur at the UFC hemi-spherical ends.

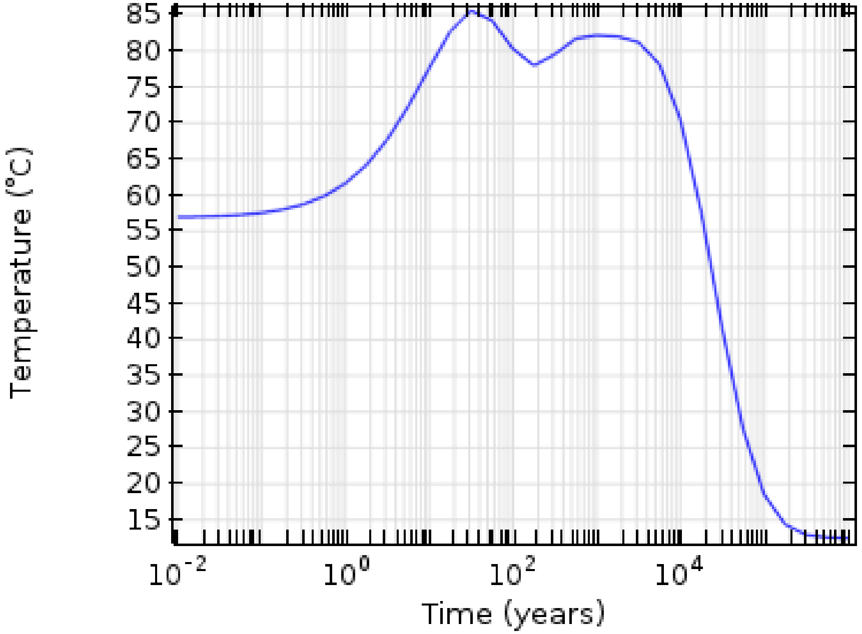
Briggs, McKelvie, Sleep and Krol, Science of Total Environment, 2017

Steady State Sulphide Transport

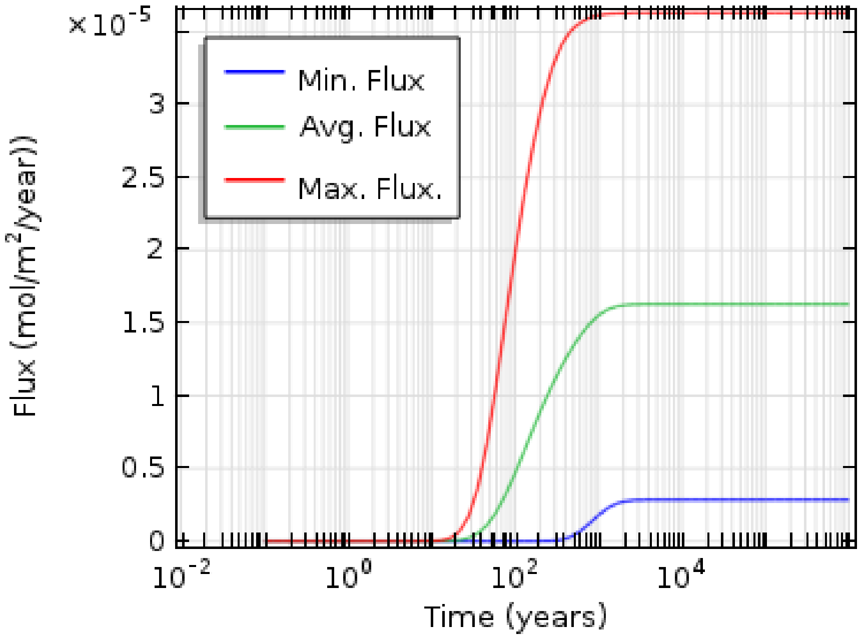
Model Type	**MIC Rate (mm per 1 million years per PPM sulphide)**
3D – UFC package – minimum *20 cm* bentonite	0.8 (average), 1.1 (max.)
3D – UFC package – minimum *30 cm* bentonite	0.65 (average), 0.86 (max.)
3D – Placement room – minimum 30 cm bentonite	**0.31 (average), 0.76 (max.)**

Thermal Sulphide Modelling

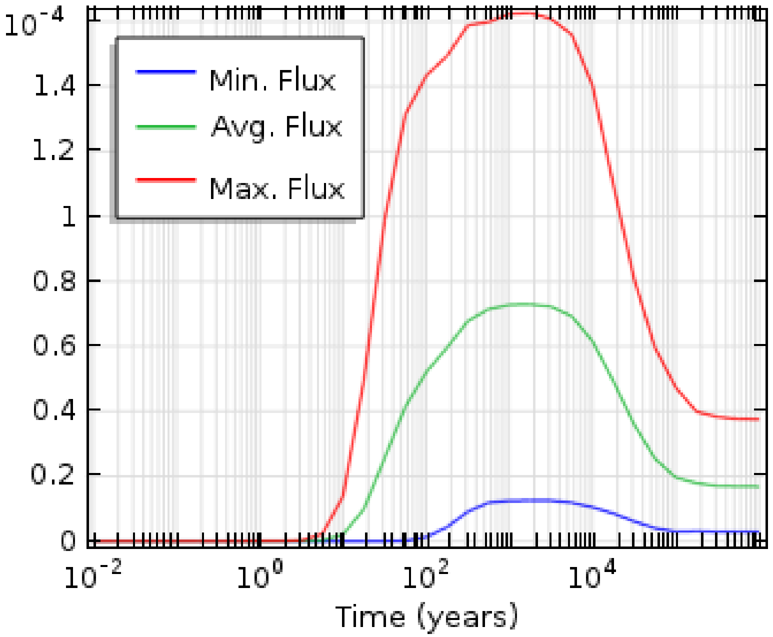
Temperature



Isothermal Case



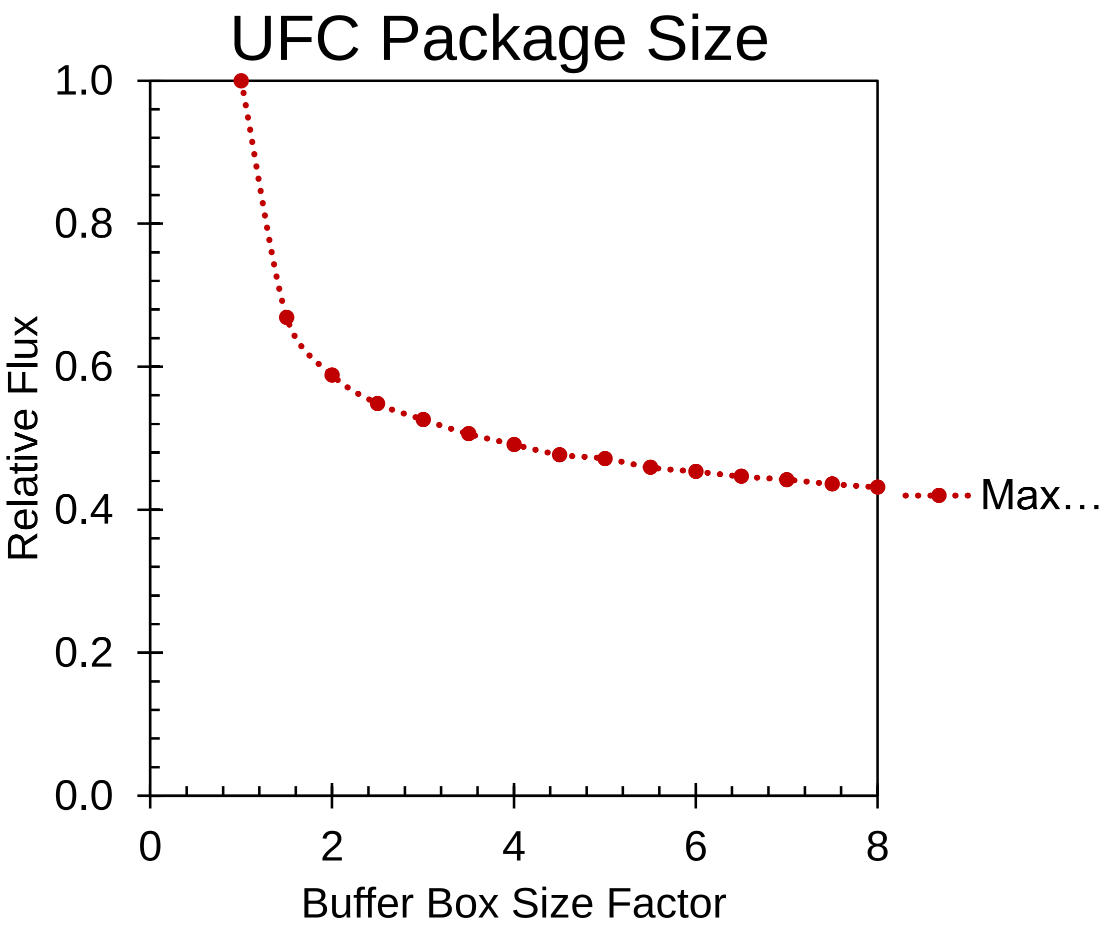
Thermal Case

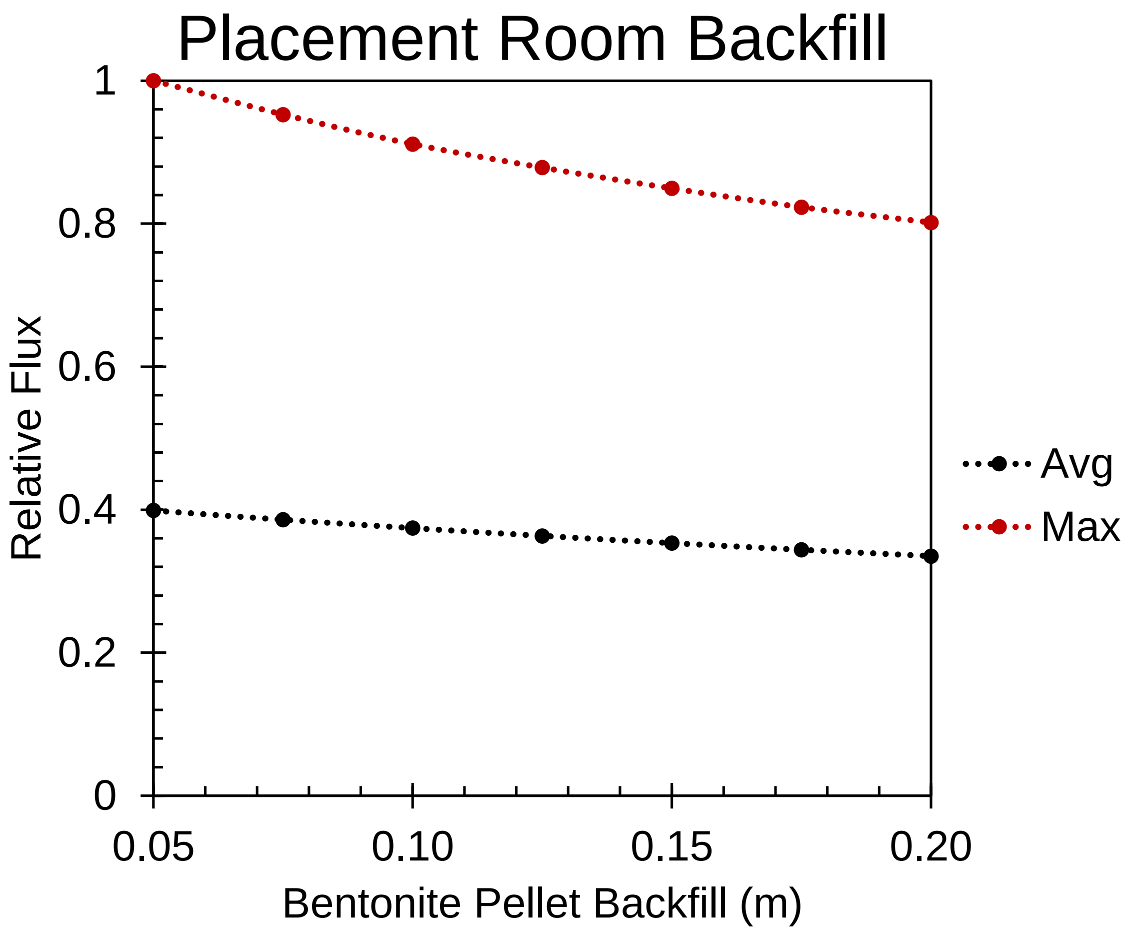


Maximum corrosion rates:

- Isothermal case at 25°C: 0.77 mm/1 million years/ppm sulphide
- Isothermal case at 11°C: 0.52 mm/1 million years/ppm sulphide
- Thermal case (cumulative): 0.60 mm total over 1 million years (per ppm sulphide)

Sensitivity Analysis – Bentonite Thickness





Sulphide Transport Modelling - Summary

- Steady state isothermal and transient thermal analysis
- Sensitivity analysis of:
  - Concentration gradient – **linear dependence**
  - Diffusion coefficient – **linear dependence**
  - Buffer box size (bentonite thickness) – **non-linear dependence**

- Localized sulphide fluxes may be higher than average rates or those predicted by 1D models due to the UFC geometry and the inclusion of 3D diffusive transport modelling.
- **The developed model can aid in the safety assessment of the UFC copper coating.**

Thank you

Acknowledgements:

- Research reported in this publication was supported by MITACS and NWMO who provide project funding through York University

Extra Slides

Effective Diffusion Coefficient

- D_{eff} is the effective diffusion coefficient at 25°C: 1x10^{-11} m^2/s

$$D_{eff} = \tau\theta_{eff}D_w$$

where ….

- D_w is the diffusion coefficient of sulphide in water (Chemistry Handbook, 2009),
- The tortuosity (τ) is assumed to 0.1 (Oscarson et al. 1994) and
- Total porosity is assumed to be a sum of accessible and non-accessible pores and the accessible pores are further broken into transport porosity and storage porosity. We assume an transport porosity = 0.1