U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Clean. Reliable. Nuclear.

GDSA Development and International Collaboration

U.S. Nuclear Waste Technical Review Board, Fact Finding Meeting
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Las Vegas, NV

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SAND2019-2043 PE

Geologic Disposal Safety Assessment (GDSA) Team

Thanks to GDSA team members

Jennifer Frederick, Glenn Hammond, Paul Mariner,
Dave Sevougian, Emily Stein

Sandia National Laboratories

And to the process modeling teams at

Los Alamos National Laboratory EST. 1943

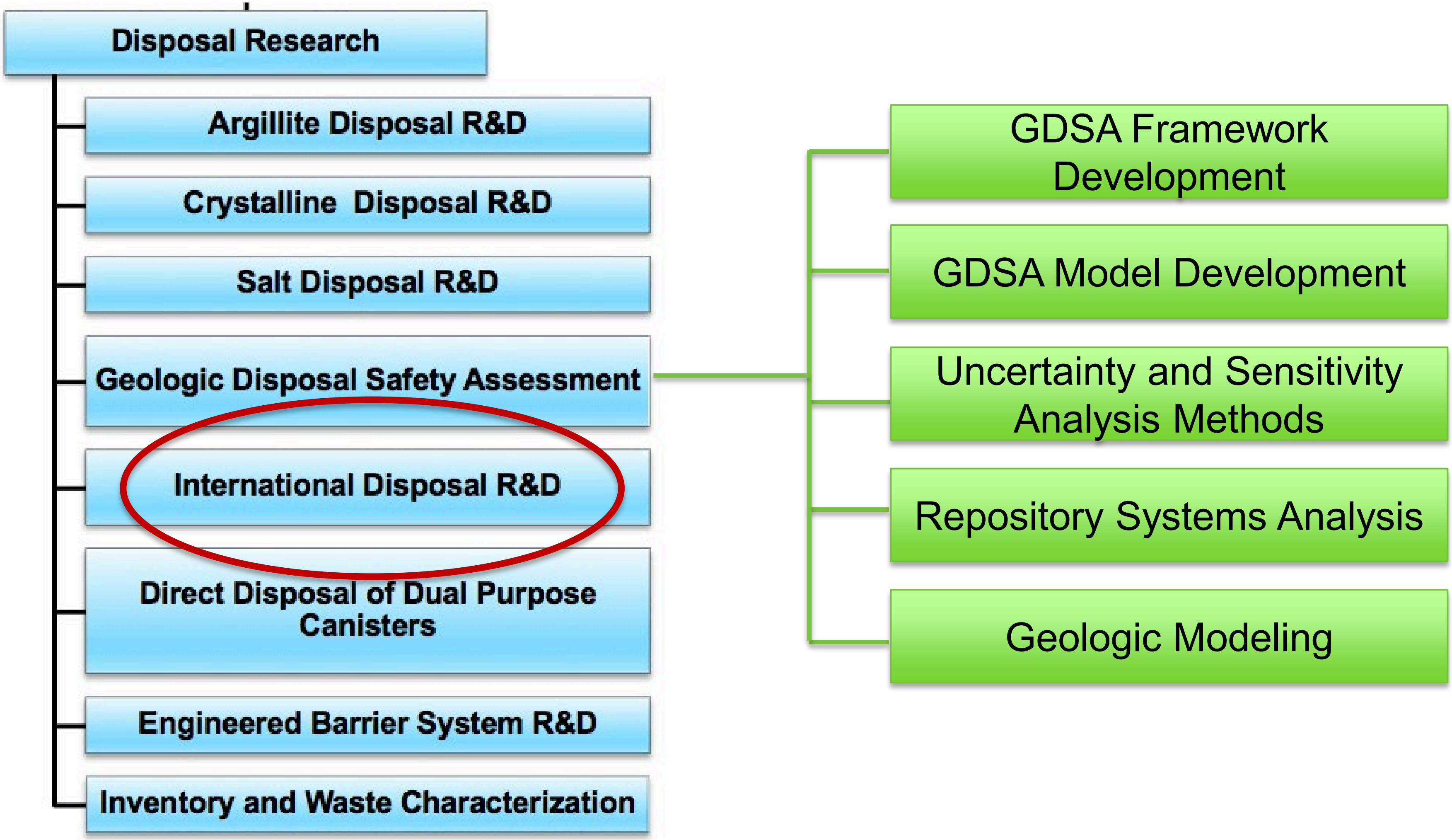
Berkeley Lab

Lawrence Livermore

Argonne National Laboratory

Pacific Northwest National Laboratory

Geologic Disposal Safety Assessment
Work Scope



How GDSA Benefits from International Collaboration

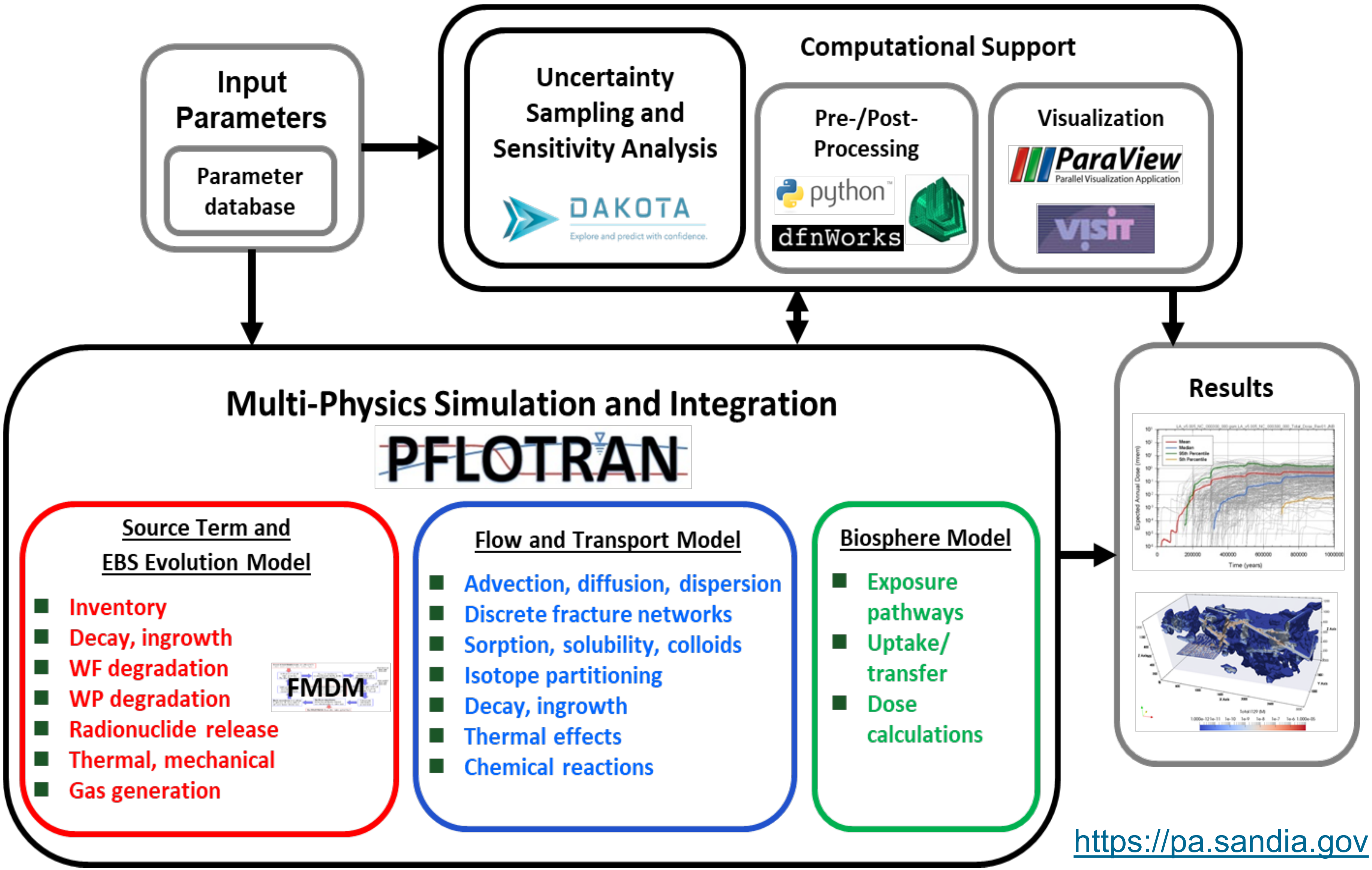
- International datasets and concepts
  - Technical bases (Natural Barrier System (NBS), Disturbed Rock Zone (DRZ), Engineered Barrier System (EBS))
- Contributions to post-closure performance assessment (PA) models
  - Analysis of Features, Events, and Processes (FEPs)
  - Process model development and validation
- Confidence enhancement
  - PA methodology (including uncertainty quantification and sensitivity analysis) in accordance with international standards of practice
  - Improve confidence in PA software through benchmarking, debugging, and demonstration on diverse problems
  - Expanded functionality through user contributions
  - State-of-the-art developments in methods and tools

Underground Research Labs (URLs) – Contributions to Post-Closure PA

Collaboration	Presenter	GDSA Integration
BRIE, GREET, LTDE	Hari Viswanathan (LANL)	Methods for computationally efficient simulation of flow and transport in fractures.
Colloid Formation and Migration at Grimsel	Hakim Boukhalfa (LANL)	Generalized model for colloid-facilitated transport.
FEBEX-DP and HotBENT	Liange Zheng (LBNL)	Process model(s) for evolution of buffer permeability, porosity, and adsorption.
WIPP and Asse Mine Salt Heater Tests	Kris Kuhlman (SNL) and Phil Stauffer (LANL)	Process model(s) for evolution of DRZ and backfill permeability and porosity in salt. Conceptual model for brine availability.
DECOVALEX gas migration in clay	Jonny Rutqvist (LBNL)	Conceptual model for gas migration in clay. Dependency of gas permeability on pressure or stress.

GDSA Framework

Comprehensive software toolkit for post-closure performance assessment



https://pa.sandia.gov

GDSA Framework

Comprehensive software toolkit for post-closure performance assessment

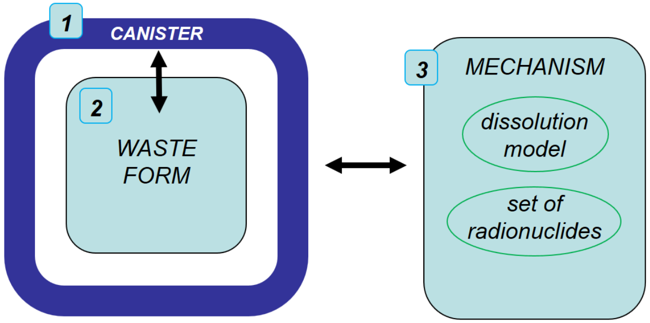
- PFLOTRAN development
  - Robust multiphase and high temperature capability
  - Coupled subsystem processes
    - Colloid stability and transport **Boukhalfa**
    - Evolution of the EBS and the DRZ **Zheng, Kuhlman/Stauffer, Rutqvist**
    - Fracture flow and transport **Viswanathan**
- Quality Assurance
  - Software verification test suite
  - Regression and unit tests
  - Documentation
- International visibility and promotion
  - Open source software development
  - PFLOTRAN short courses
  - Participation in international venues

GDSA Model Development

Supports GDSA Framework development

Concept development

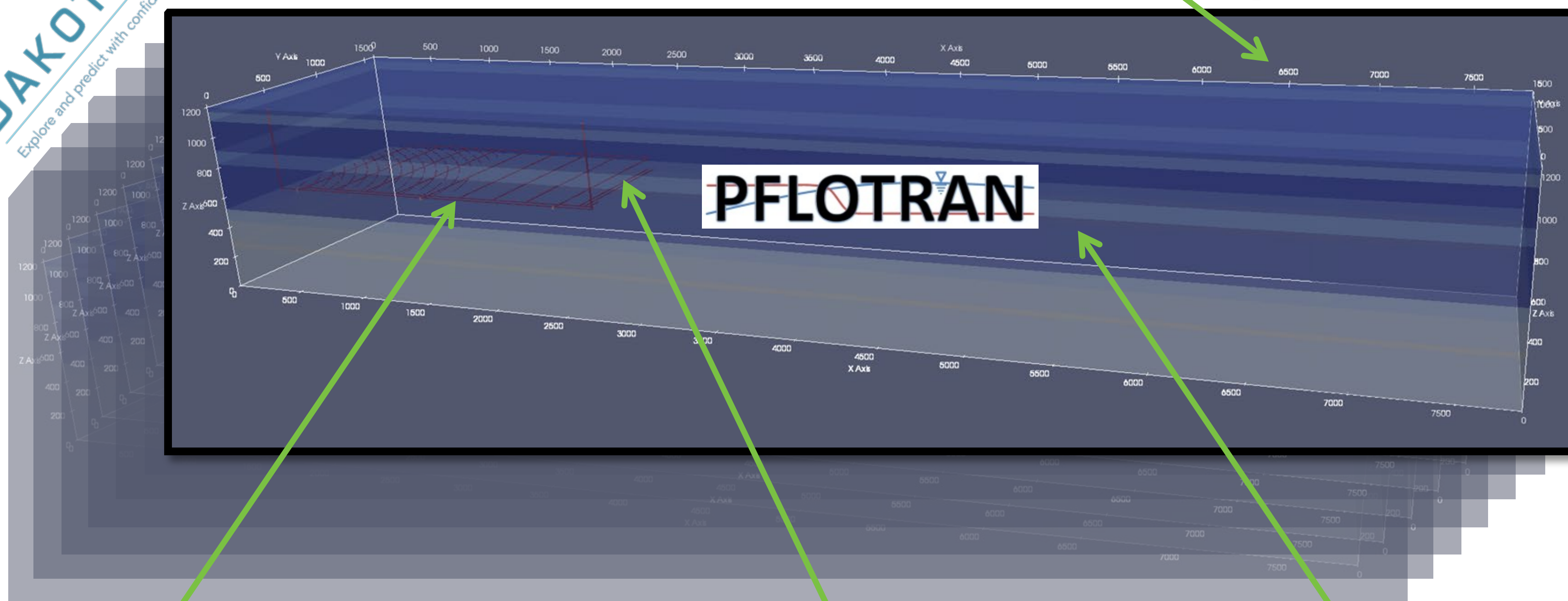
- Mechanistic approaches to waste package degradation
- Mechanistic approaches to waste form dissolution
- Source terms associated w/ Dual Purpose Canisters
  - Criticality consequence analysis
- Surrogate modeling approaches
  - Fuel Matrix Degradation Model
  - Coupled processes in the EBS **Zheng, Rutqvist**



Mariner et al. 2016

Repository Systems Analysis

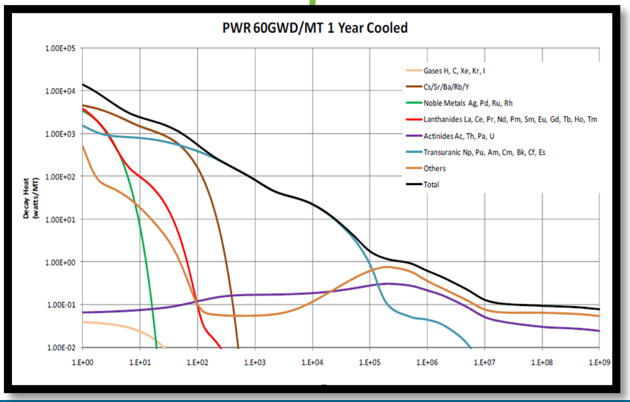
Biosphere

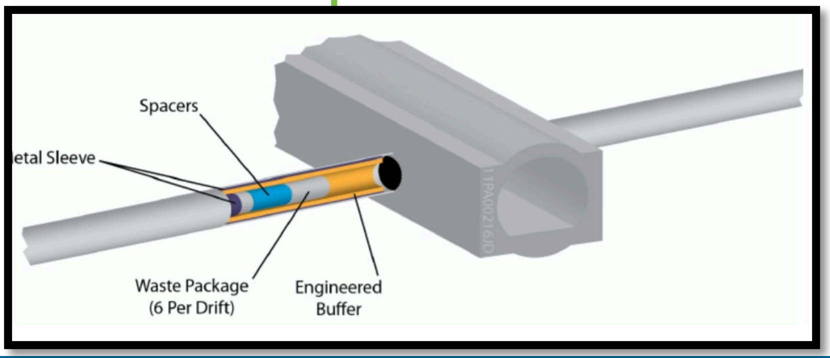


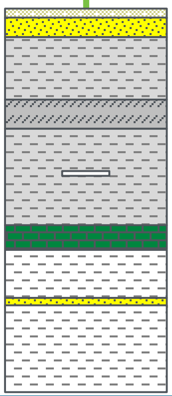
Waste Source Term

Engineered Barrier System

Natural Barrier System







Repository Systems Analysis

- Reference case concepts
  - Features/Events/Processes (FEPs)
  - Repository design/layout
  - DPC disposal concepts
  - Technical bases for engineered and natural systems
- Total system simulations and probabilistic PA
- Nearfield simulations
- Supported by Geologic Modeling
  - Geographic Information Systems
  - Geologic Framework Modeling
- Relies heavily on international datasets

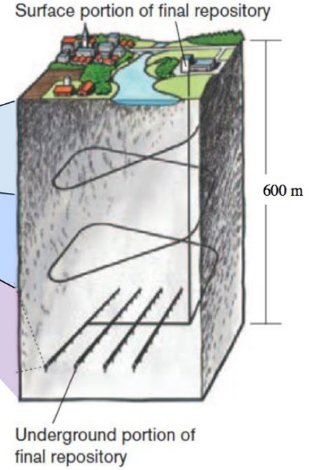
Reference Cases

1. Crystalline

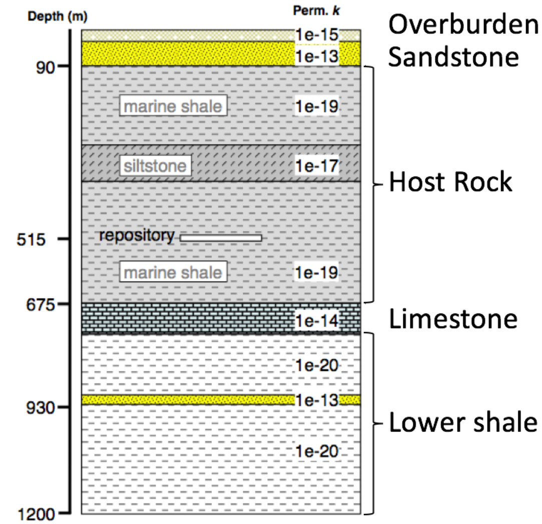
Table 2 Hydrogeological DFN parameters for each fracture domain, fracture set and depth zone

Fracture domain/elevation (m.a.s.l)[a]	Fracture set name	Orientation set pole: (trend, plunge), conc.	Size model, power-law (r_0, k_r) (m, −)	Intensity, (P_{32}), valid size interval: r_0 to 564 m (m^2/m^3)	Parameter values for the transmissivity models: Semi-correlated (a,b,σ)	Correlated (a,b)	Uncorrelated (μ,σ)
FFM01 and FFM06>−200	NS	(292, 1) 17.8	(0.038, 2.50)	0.073	$6.3 \cdot 10^{-9}$, 1.3, 1.0	$6.7 \cdot 10^{-9}$, 1.4	−6.7, 1.2
	NE	(326, 2) 14.3	(0.038, 2.70)	0.319			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.107			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.088			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.543			
FFM01 and FFM06 −200 to −400	NS	(292, 1) 17.8	(0.038, 2.50)	0.142	$1.3 \cdot 10^{-9}$, 0.5, 1.0	$1.6 \cdot 10^{-9}$, 0.8	−7.5, 0.8
	NE	(326, 2) 14.3	(0.038, 2.70)	0.345			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.133			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.081			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.316			
FFM01 and FFM06<−400	NS	(292, 1) 17.8	(0.038, 2.50)	0.094	$5.3 \cdot 10^{-11}$, 0.5, 1.0	$1.8 \cdot 10^{-10}$, 1.0	−8.8, 1.0
	NE	(326, 2) 14.3	(0.038, 2.70)	0.163			
	NW	(60, 6) 12.9	(0.038, 3.10)	0.098			
	EW	(15, 2) 14.0	(0.038, 3.10)	0.039			
	HZ	(5, 86) 15.2	(0.038, 2.38)	0.141			
FFM02>−200	NS	(83, 10) 16.9	(0.038, 2.75)	0.342	$9.0 \cdot 10^{-9}$, 0.7, 1.0	$5.0 \cdot 10^{-9}$, 1.2	−7.1, 1.1
	NE	(143, 9) 11.7	(0.038, 2.62)	0.752			
	NW	(51, 15) 12.1	(0.038, 3.20)	0.335			
	EW	(12, 0) 13.3	(0.038, 3.40)	0.156			
	HZ	(71, 87) 20.4	(0.038, 2.58)	1.582			
FFM03, FFM04 and FFM05>−400	NS	(292, 1) 17.8	(0.038, 2.60)	0.091	$1.3 \cdot 10^{-8}$, 0.4, 0.8	$1.4 \cdot 10^{-8}$, 0.6	−7.2, 0.8
	NE	(326, 2) 14.3	(0.038, 2.50)	0.253			
	NW	(60, 6) 12.9	(0.038, 2.55)	0.258			
	EW	(15, 2) 14.0	(0.038, 2.40)	0.097			
	HZ	(5, 86) 15.2	(0.038, 2.55)	0.397			
FFM03, FFM04 and FFM05<−400	NS	(292, 1) 17.8	(0.038, 2.60)	0.102	$1.8 \cdot 10^{-8}$, 0.3, 0.5	$7.1 \cdot 10^{-9}$, 0.6	−7.2, 0.8
	NE	(326, 2) 14.3	(0.038, 2.50)	0.247			
	NW	(60, 6) 12.9	(0.038, 2.55)	0.103			
	EW	(15, 2) 14.0	(0.038, 2.40)	0.068			
	HZ	(5, 86) 15.2	(0.038, 2.55)	0.250			

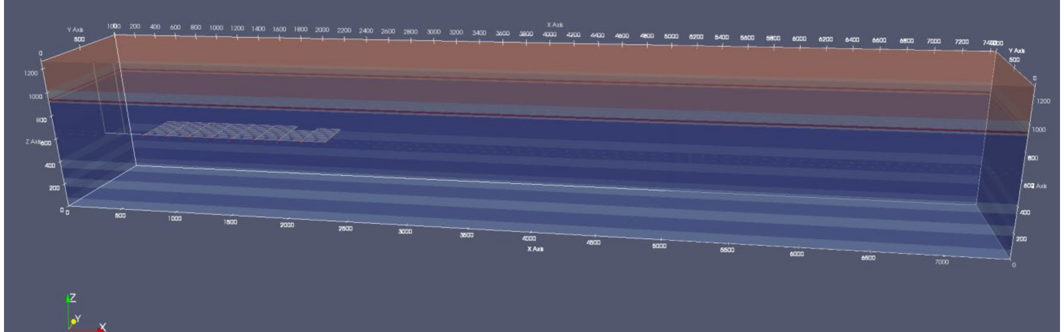
[a] Meters above sea level



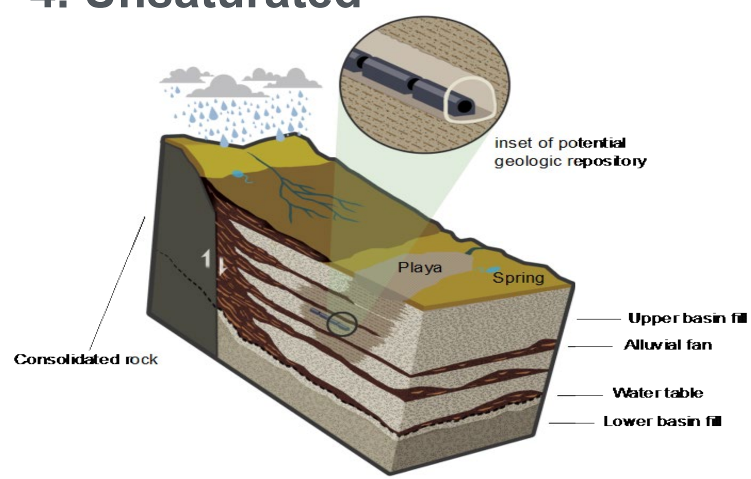
2. Shale



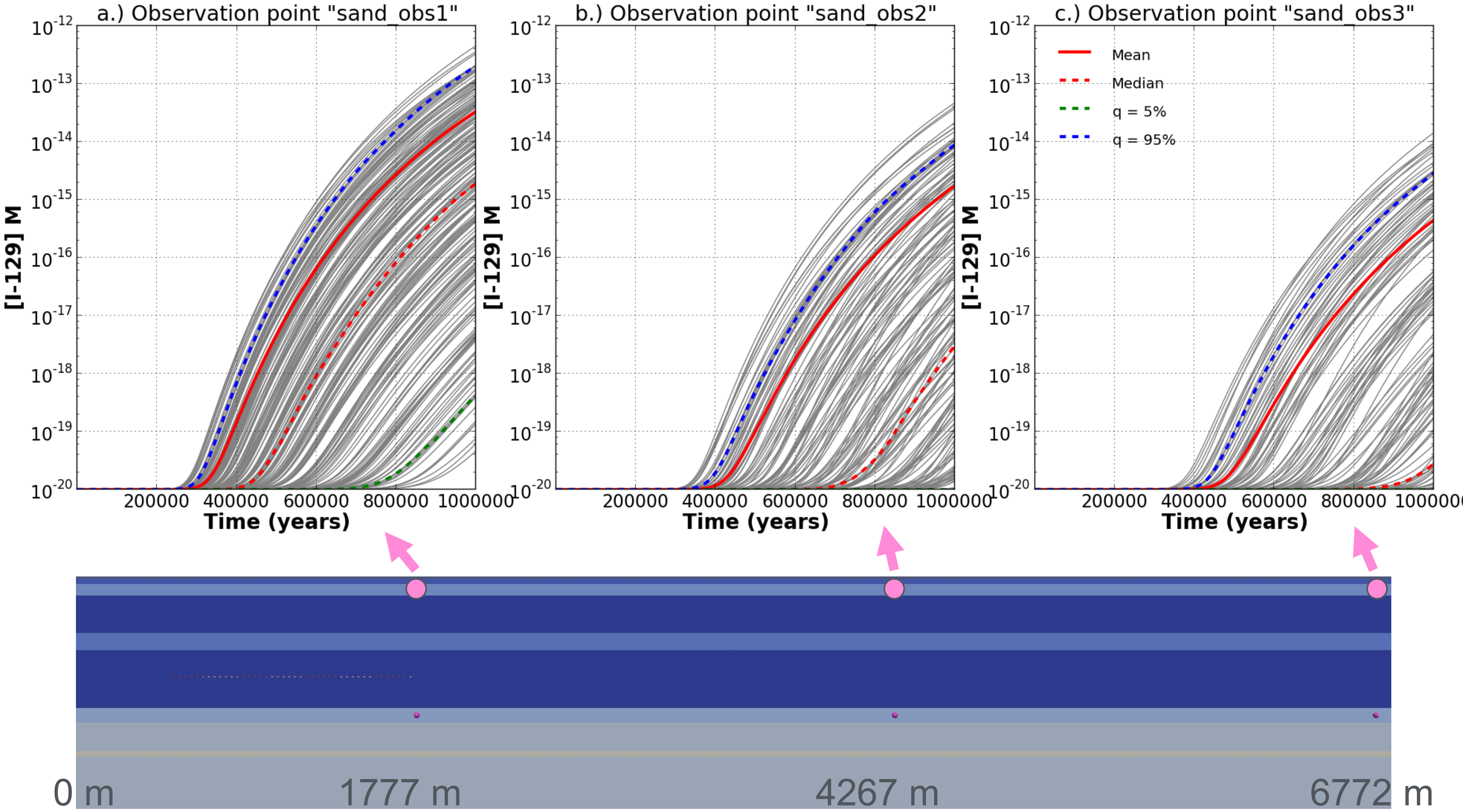
3. Salt



4. Unsaturated



Uncertainty Quantification and Sensitivity Analysis (UQ/SA)



Uncertainty Quantification and Sensitivity Analysis (UQ/SA)

- Implementation of traditional and new UQ/SA methods
  - Partial correlation, stepwise regression, rank transform
  - Variance decomposition via polynomial chaos expansion, Gaussian process, etc.
  - Efficient methods for computationally expensive problems
- Application of methods to reference cases
  - Which methods are best for which problems?
  - Inform research and development (R&D) activities through identification of influential inputs
- International collaboration (informal group)
  - Develop joint approach to sensitivity analysis
  - Exchange knowledge
  - Comparison of software and methods on variety of problems

1. Introduction, Purpose, and Context

2. Safety Strategy

2.1 Management Strategy

a. Organizational/mgmt. structure
b. Safety culture & QA
c. Planning and Work Control
d. Knowledge management
e. Oversight groups

2.2 Siting & Design Strategy

a. National laws
b. Site selection basis & robustness
c. Design requirements
d. Disposal concepts
e. Intergenerational equity

2.3 Assessment Strategy

a. Regulations and rules
b. Performance goals/safety criteria
c. Safety functions/multiple barriers
d. Uncertainty characterization
e. RD&D prioritization guidance

3. Technical Bases

3.1 Site Selection

a. Siting methodology
b. Repository concept selection
c. FEPs Identification
d. Technology development
e. Transportation considerations
f. Integration with storage facilities

3.2 Pre-closure Basis

a. Repository design & layout
b. Waste package design
c. Construction requirements & schedule
d. Operations & surface facility
e. Waste acceptance criteria
f. Impact of pre-closure activities on post-closure

3.3 Post-closure Bases (FEPs)

3.3.1 Waste & Engineered Barriers Technical Basis

a. Inventory characterization
b. WF/WP technical basis
c. Buffer/backfill technical basis
d. Shafts/seals technical basis
e. UQ (aleatory, epistemic)

3.3.2 Geosphere/ Natural Barriers Technical Basis

a. Site characterization
b. Host rock/DRZ technical basis
c. Aquifer/other geologic units technical basis
d. UQ (aleatory, epistemic)

3.3.3 Biosphere Technical Basis

a. Biosphere & surface environment:
- Surface environment
- Flora & fauna
- Human behavior

4. Disposal System Safety Evaluation

4.1 Pre-closure Safety Analysis

a. Surface facilities and packaging
b. Mining and drilling
c. Underground transfer and handling
d. Emplacement operations
e. Design basis events & probabilities
f. Pre-closure model/software validation
g. Criticality analyses
h. Dose/consequence analyses

4.2 Post-closure Safety Assessment

a. FEPs analysis/screening
b. Scenario construction/screening
c. PA model/software validation
d. Barrier/safety function analyses and subsystem analyses
e. PA and Process Model Analyses/Results
f. Uncertainty characterization and analysis
g. Sensitivity analyses

4.3 Confidence Enhancement

a. R&D prioritization
b. Natural/anthropogenic analogues
c. URL & large-scale demonstrations
d. Monitoring and performance confirmation
e. International collaboration & peer review
f. Verification, validation, transparency
g. Qualitative and robustness arguments

5. Synthesis & Conclusions

a. Key findings and statement(s) of confidence
b. Discussion/disposition of remaining uncertainties
c. Path forward

Safety Case Component 3: Technical Bases

3.3 Post-closure Bases (FEPs)

3.3.1 Waste & Engineered Barriers Technical Basis

a. Inventory characterization
b. Waste form/waste package technical basis
c. Buffer/backfill technical basis
d. Shafts/seals technical basis
e. UQ (aleatory, epistemic)

3.3.2 Geosphere/ Natural Barriers Technical Basis

a. Site characterization
b. Host rock/DRZ technical basis
c. Aquifer/other geologic units technical basis
d. UQ (aleatory, epistemic)

International datasets contribute to GDSA generic reference cases.

Crystalline Reference Case – Natural Barrier System Technical Basis

Feature, Process	International Influences	URL / Site	References
Reference case site concept	Sweden	Forsmark	SKB 2007; 2008 Mariner et al. 2016
Fracture distribution and properties	Sweden	Forsmark	Follin et al. 2014; Joyce et al. 2014; Wang et al. 2014; Mariner et al. 2016
Crystalline matrix permeability and porosity	Switzerland, Canada, Korea	Grimsel, Lac du Bonnet, KURT	Schild et al. 2001; Martino & Chandler 2004; Cho et al. 2013; Mariner et al. 2016
Effective diffusion coefficient	Switzerland	Grimsel	Soler et al. 2015; Mariner et al. 2016
DRZ permeability and extent	Canada, Korea	Lac du Bonnet, KURT	Martino & Chandler 2004; Cho et al. 2013; Mariner et al. 2016
Geochemical Environment	Sweden, Finland, Canada	Olkiluoto, Forsmark, etc.	Posiva 2010; SKB 2006; Mariner et al. 2011

Viswanathan

Crystalline Reference Case – Engineered Barrier System Technical Basis

Feature, Process	International Influences	References
Spent Nuclear Fuel Dissolution	Sweden	SKB 2006; Sassani et al. 2016
Bentonite Buffer Concepts	Korea, etc.	Choi and Choi 2008; Wang et al. 2014; Mariner et al. 2016
Bentonite Thermal Conductivity	Germany, China	Jobmann & Buntebarth 2009; Wang et al. 2015; Mariner et al. 2016
Bentonite Porosity and Permeability	France	Liu et al. 2016; Mariner et al. 2016
Bentonite Adsorption Distribution Coefficients (K_ds)	Sweden	SKB 2004; Mariner et al. 2011

Safety Case Component 4:
Disposal System Safety Evaluation

4.2 Post-closure Safety Assessment

a. FEPs analysis/screening
b. Scenario construction/screening
c. PA model/software validation
d. Barrier/safety function analyses and subsystem analyses
e. PA and Process Model Analyses/Results
f. Uncertainty characterization and analysis
g. Sensitivity analyses

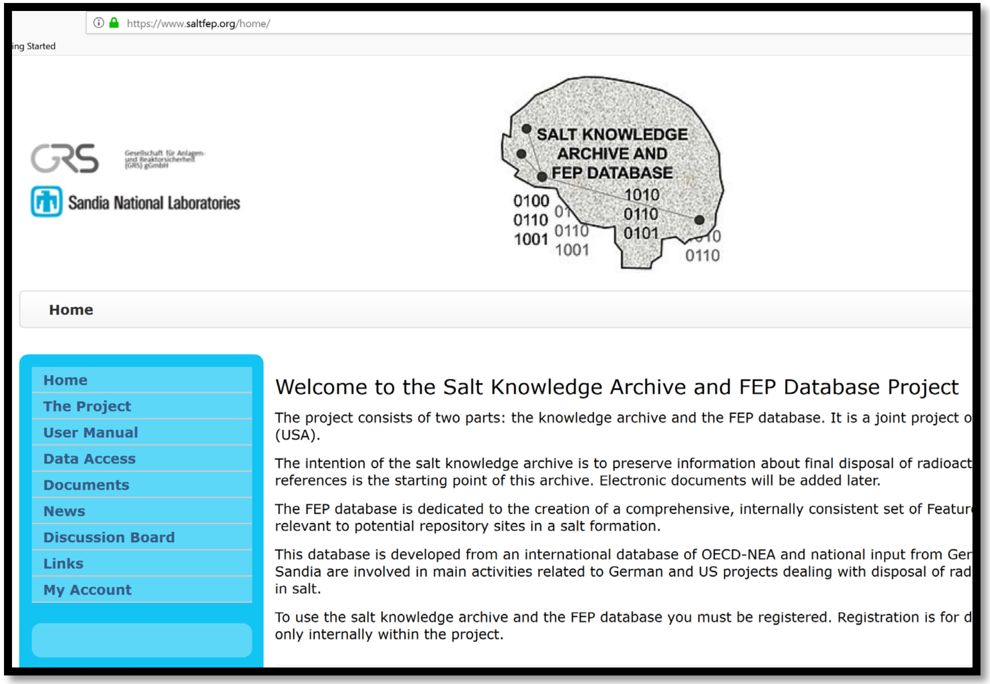
International collaboration contributes directly to GDSA models and concepts.

International collaboration increases confidence in GDSA tools and methods.

Salt Reference Case – U.S./Germany Salt FEP Collaboration

What it is:

- Common FEP list
- Refined FEP matrix approach
- Consistent with Nuclear Energy Agency (NEA) FEP database



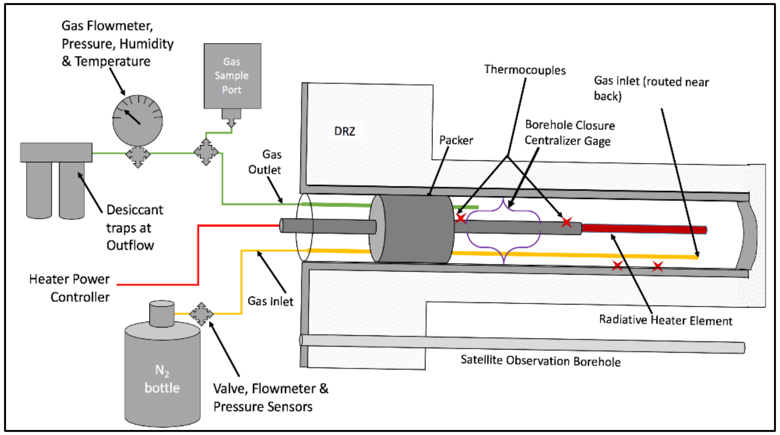
How GDSA benefits:

- Direct inclusion in salt safety case
- Applicable to all potential salt concepts
- Improves transparency and confidence

Salt Reference Case – Brine Availability Test in Salt

What it is:

- Heater test in the Waste Isolation Pilot Plant (WIPP)
- Investigate thermal effects on salt creep, evolution of porosity and permeability, gas and brine migration



Courtesy of Kris Kuhlman

How GDSA benefits:

- Improved conceptual model of Thermal-Hydro-Mechanical-Chemical (THMC) coupled processes affecting DRZ evolution
- Process model integration and/or informed PA modeling approach

Kuhlman and Stauffer

Crystalline Reference Case – Grimsel Test Site, Colloid Formation and Migration

What it is:

- Series of colloidal transport experiments at Grimsel Test Site and related laboratory experiments

How GDSA benefits:

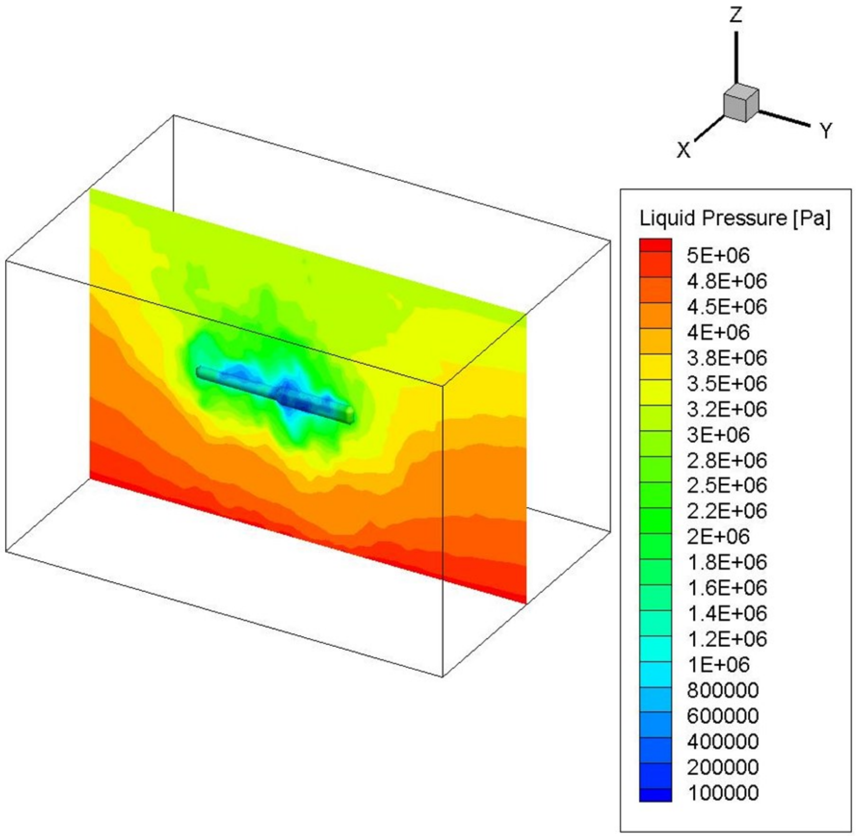
- Identify processes that result in significant colloid-facilitated transport over long time and distance scales
- Integration of generalized colloidal transport model

Boukhalfa

Crystalline Reference Case – GREET, BRIE, LTDE

What it is:

- Groundwater Recovery Experiment in Tunnel (GREET) in the Mizunami URL
- Bentonite Rock Interaction Experiment (BRIE) in the Äspö HRL
- Long Term Diffusion Experiment (LTDE) at Grimsel Test Site



Courtesy of Teklu Hadgu

How GDSA benefits:

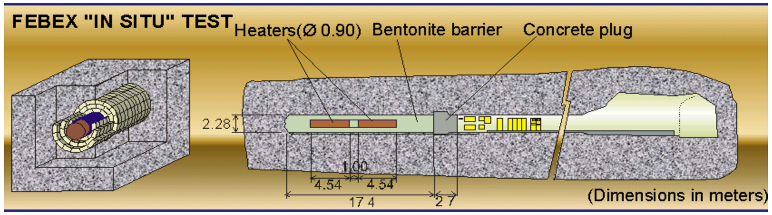
- Methods and best practices for accurate simulation of flow and transport in fractures

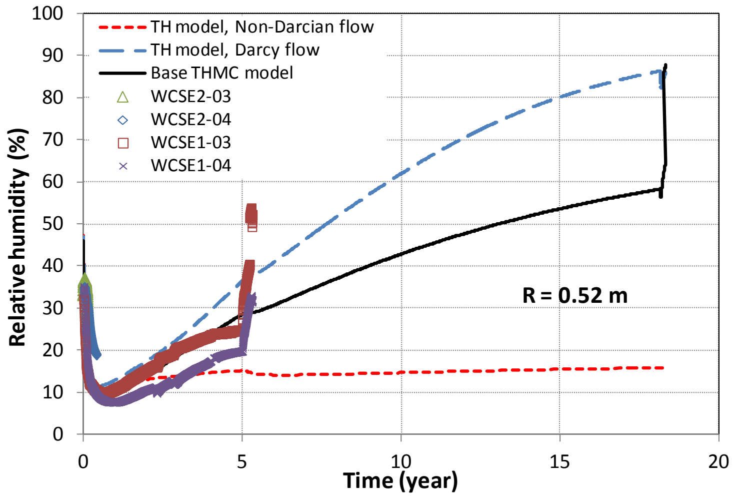
Viswanathan

Engineered Barrier System – FEBEX-DP and HotBENT

What it is:

- Heater tests in bentonite buffer at Grimsel Test Site
- Temperatures up to 100º and 200º C
- Associated THMC modeling of buffer evolution





Courtesy of Liange Zheng

How GDSA benefits:

- Identify key processes and parameters affecting evolution of buffer
- Integration of surrogate model(s) for THMC evolution of the buffer
- Thermal limits for buffer integrity

Zheng

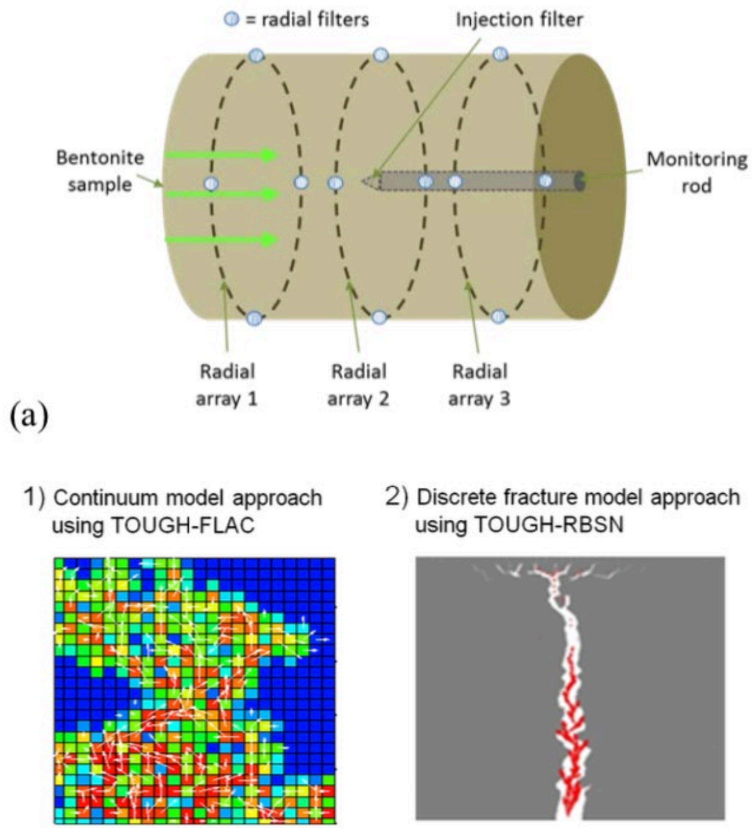
Engineered Barrier System – DECOVALEX gas migration

What it is:

- Gas injection experiment in low-permeability porous media (bentonite, shale)
- Conceptual and numerical model development and benchmarking

How GDSA benefits:

- Conceptual model for propagation of dilatant pathways in clay
- Model for dependence of gas permeability on pressure (or stress)



Rutqvist et al. 2018

Rutqvist

4. Disposal System Safety Evaluation

4.3 Confidence Enhancement

a. R&D prioritization
b. Natural/anthropogenic analogues
c. URL & large-scale demonstrations
d. Monitoring and performance confirmation
e. International collaboration & peer review
f. Verification, validation, transparency
g. Qualitative and robustness arguments

International collaboration increases confidence in GDSA tools and methods.

Sensitivity Analysis in PA: Towards a Joint Approach

- Develop international standards for best practices
- Benchmark software and methods on a variety of reference repositories
- Informal collaboration with participants from:

Sandia National Laboratories

SCK•CEN
STUDIECENTRUM VOOR KERNENERGIE
CENTRE D'ETUDE DE L'ENERGIE NUCLEAIRE

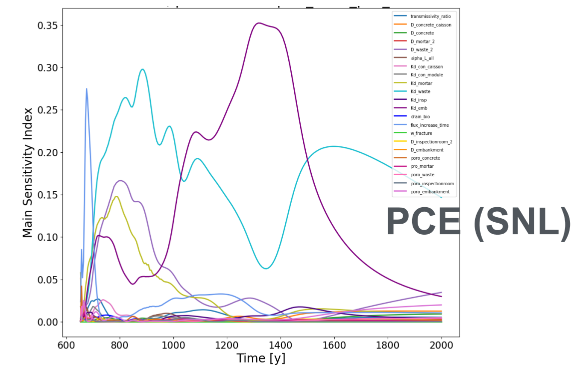
TU Clausthal

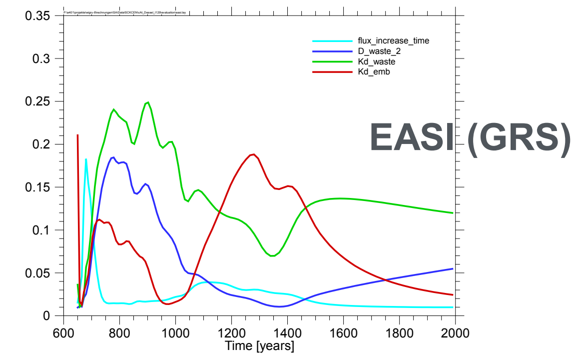
POSIVA

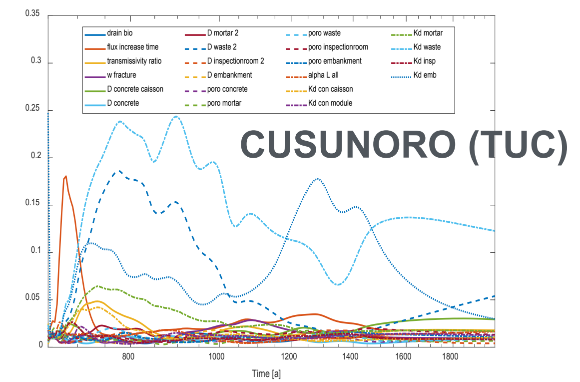
GRS

And growing…

Rohlig et al. 2018







DECOVALEX 2023 – PA Benchmark Potential Tasks

- **Task 1: Problem definition**
  Choice of host rock(s) and repository design, and development of reference case(s). Reference case(s) will be agreed upon by participating countries and will be such that all countries can model & analyze with their tools.
- **Task 2: Model Setup**
  Development of forward models for generic reference case(s). Setup of uncertainty sampling and sensitivity analysis framework. Each modeling group uses its own the PA codes/software.
- **Task 3: Sensitivities**
  Evaluation of sensitivity metrics for selected key parameters. Comparison of sensitivity analyses (SA) methods and metrics.
- **Task 4: PA Modeling and UQ**
  Evaluation of parameter uncertainty: Performance assessment simulations for a defined set of uncertain parameters and their uncertainty ranges, for defined metrics such as dose to an individual or aqueous-phase concentration of agreed-upon radionuclides.
- **Task 5: Conceptual Model Uncertainty**
  Evaluation of conceptual model uncertainty: Use of mechanistic models versus surrogate or reduced order models. Also methods of propagating uncertainty from one submodel to another.
- **Task 6: Synthesis**
  Synthesis and guidance: How simple or complex should PA be; conservatism vs realism, risk dilution; scenario lumping or separate scenario assessment; total PA vs. assessment of individual barriers; etc.

How GDSA Benefits from International Collaboration

- Use international datasets and concepts
  - Technical bases (NBS/DRZ/EBS)
- Direct contributions to post-closure PA
  - FEPs analysis
  - Process model development and validation
- Confidence enhancement
  - PA methodology (including UQ/SA) in accordance with international standards of practice
  - Improve confidence in PA software through benchmarking, debugging, and demonstration on diverse problems
  - Expanded functionality through user contributions
  - Stay abreast of state-of-the-art developments in methods and tools

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Questions?

Clean. **Reliable. Nuclear.**

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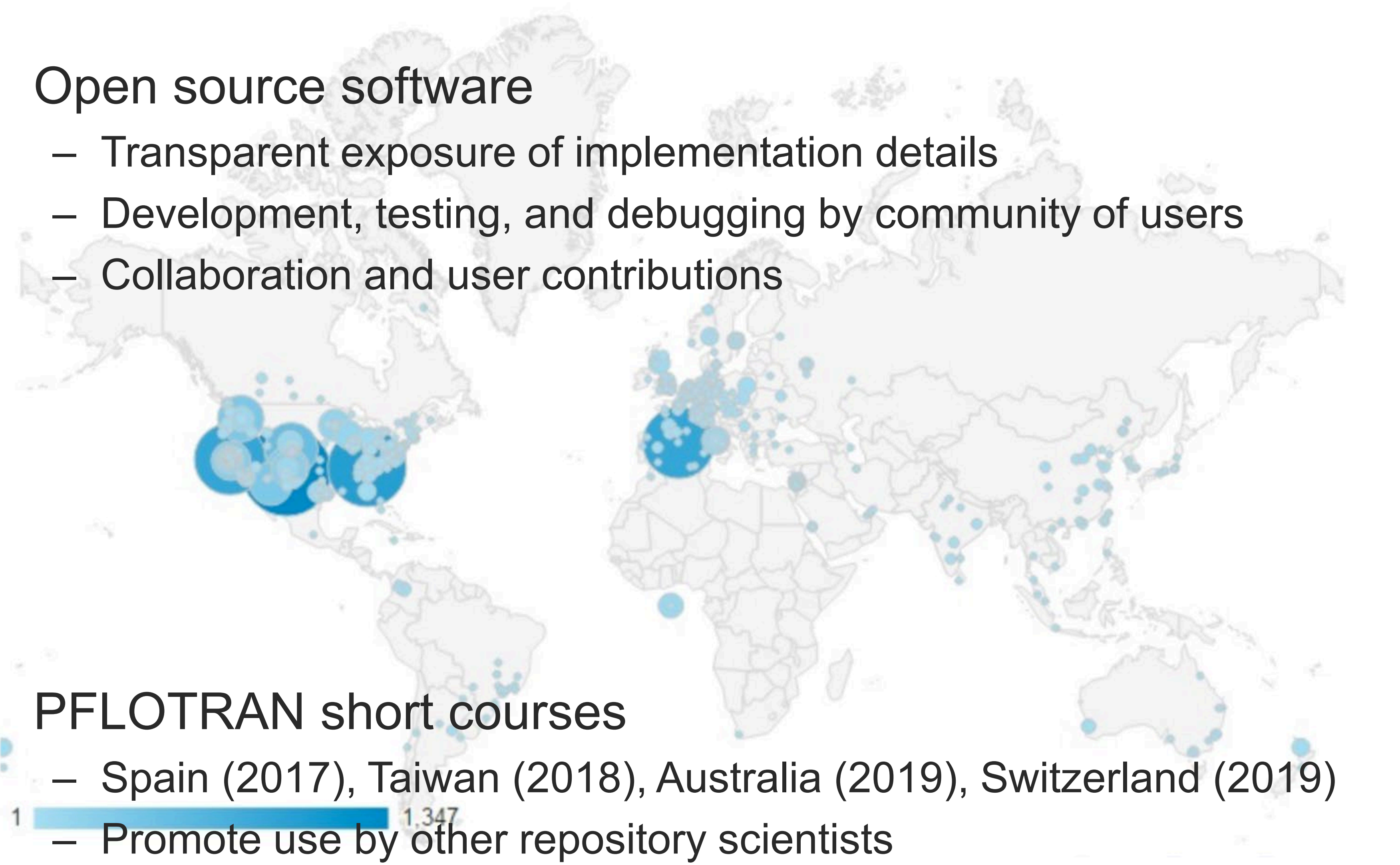
Backup Slides

Shale Reference Case – NBS & EBS Technical Bases

Feature, Process	International Influences	URL / Site	References
Shale Tortuosity	Switzerland	Mont Terri	Van Loon & Mibus 2015; Mariner et al. 2017
Geochemical Environment	France, Switzerland	Bure, Mont Terri	ANDRA 2005; Turrero et al. 2006; Jove Colon et al. 2014
Disposal concepts	France	Bure	ANDRA 2005; Hardin and Kalinina 2016
SNF dissolution	Sweden		SKB 2006; Sassani et al. 2016
Bentonite concepts and properties	Korea, Germany, China, France		Choi and Choi 2008; Jobmann & Buntebarth 2009; Liu et al. 2016; Wang et al. 2015; Jove Colon et al. 2014; Mariner et al. 2017
Bentonite K_ds	France	Bure	ANDRA 2005; Clayton 2011

PFLOTRAN International Outreach

- Open source software
  - Transparent exposure of implementation details
  - Development, testing, and debugging by community of users
  - Collaboration and user contributions



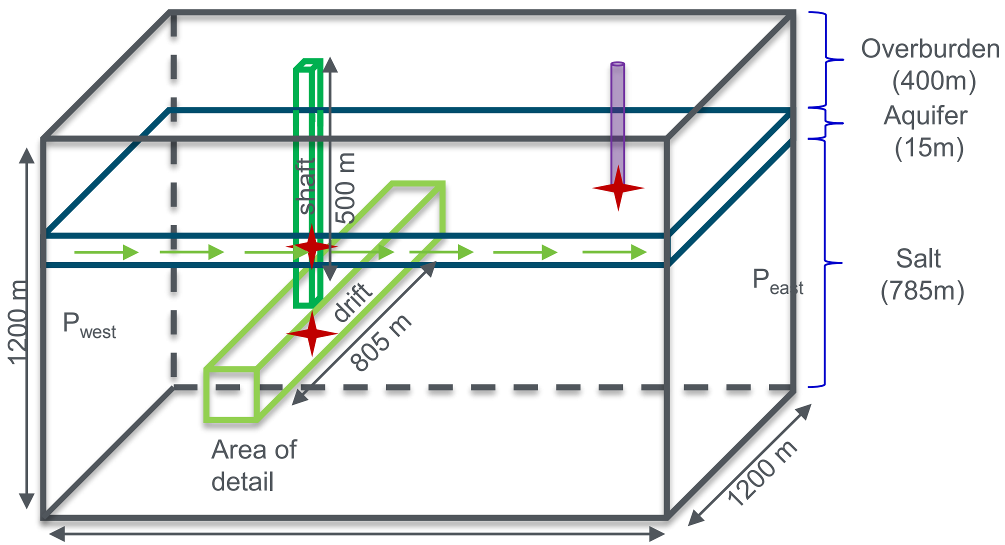
- PFLOTRAN short courses
  - Spain (2017), Taiwan (2018), Australia (2019), Switzerland (2019)
  - Promote use by other repository scientists
  - Grow community of users

U.S./Germany Salt PA Code Comparison

- Compare alternative representations
- Verify software functionality
- Identify needed simulation capabilities

PFLOTRAN

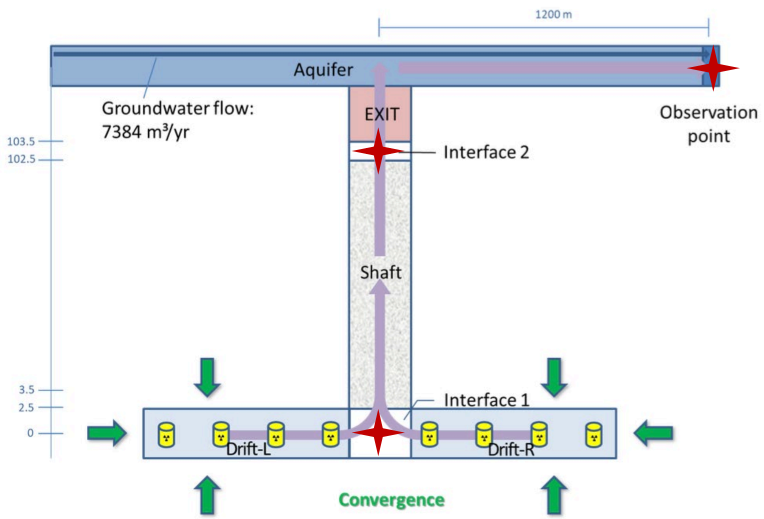
- 3-D



Courtesy of Jenn Frederick

RepoTREND

- Linked 1-D



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