U.S. Progress in Geologic Disposal Safety Assessment (GDSA) Framework

Geoff Freeze and Emily Stein

Sandia National Laboratories

SAND2019-xxxx PE

SFWD

Spent Fuel & Waste Disposition

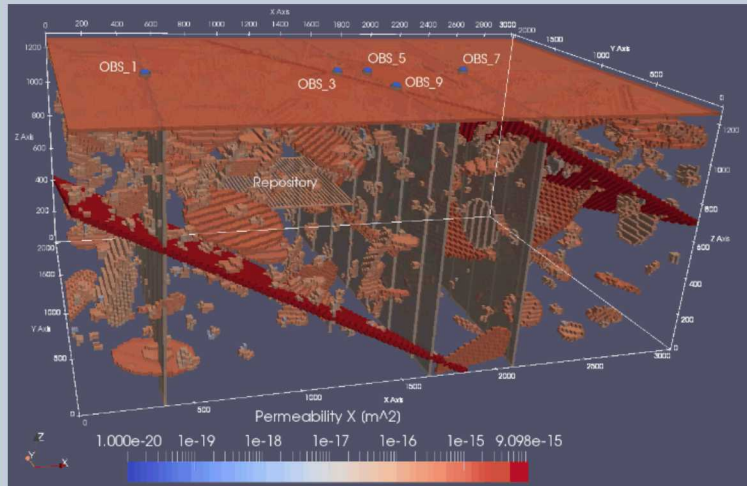
High Level Bilateral Commission (HLBC)

Spent Fuel Management Working Group Workshop

Argonne National Laboratory – *Lemont, Illinois*

July 16-18, 2019

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

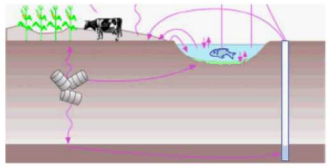


JOINT RESEARCH PROPOSAL 3

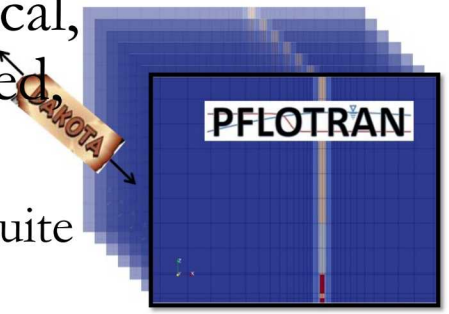
- Development of Safety Assessment Code for the Spent Nuclear Fuel Repository
  - Develop performance assessment (PA) technologies and codes to support:
    - Conceptual design parameters for disposal
    - Development of a safety case that incorporates coupled thermal-hydrologic-mechanical-chemical (THMC) processes
  - Important factors include:
    - Evaluation of candidate engineered barrier materials, including thermal effects
    - Evaluation of natural barriers for deep mined disposal

Recent U.S. Research on Development of Safety Assessment Codes

- DOE funding for advanced PA modeling began in 2009 as part of the Used Fuel Disposition Campaign (UFDC), which was re-organized in 2017 into Spent Fuel and Waste Disposition (SFWD)
  - **(2010 - 2012)** Developed the Generic Performance Assessment Model (GPAM) for application to mined repositories and deep borehole disposal
    - GPAM is based on commercial GoldSim software
  - **(2013 - Present)** Developing a new Geologic Disposal Safety Assessment (GDSA) modeling capability that implicitly couples thermal, hydrological, chemical and mechanical phenomena using advanced high-performance computing (HPC) platforms
    - GDSA is based on the open-source PFLOTRAN code suite



GoldSim
TECHNOLOGY GROUP



U.S. – ROK Technical Engagement in PA Modeling

- (2011 - 2016) Joint Fuel Cycle Studies (JFCS)
  - Status updates and information exchange (technical reports)
  - Collaborative development of GPAM (GoldSim) test problem
    - Daejeon, Korea (March 2012)
    - Albuquerque, NM, USA (June 2012)
    - Daejeon, Korea (March 2013)
  - Development of GDSA (PFLOTRAN)
    - Richland, WA, USA (June 2014)
    - Jeju, Korea (April 2015)
- (2017 – Present) High Level Bilateral Commission (HLBC)
  - Continued development of GDSA (PFLOTRAN)
    - Gwacheon, Korea (June 2017)

U.S. – ROK Recent Information Exchange in PA Modeling

#	Provider	Topical Area	Document Title of Deliverable	Status	ID
1	USA (G. Freeze)	1 - Evaluation Tools	PA Modeling and Sensitivity Analysis of Generic Disposal System Concepts, FCRD-UFD-2014-000320, SAND2014-17658, September 2014	Delivered to ROK on November 24, 2014 (by email)	1.1-A
2	USA (G. Freeze)	1 - Evaluation Tools	Nuclear Fuels Storage and Transportation Planning Project Inventory Basis (FCRD-NFST-2013-000263 Rev 1) The above report was sent in place of "UFDC Inventory Report (FCRD-USED-2010-000031 Rev 5)" because it contains more recent information.	Delivered to ROK on November 17, 2014 (by email)	1.1-B
3	USA (G. Freeze)	1 - Evaluation Tools	YMP License Application (LA) Safety Analysis report (SAR) Chapter 2 (Repository Safety After Permanent Closure), describing flow and transport in the unsaturated zone (UZ) and saturated zone (SZ) and the implementation of these process models in PA.	Delivered to ROK on September 5, 2014 (by link to NRC website)	1.1-C
4	USA (G. Freeze)	1 - Evaluation Tools	UFDC GDSA end of FY 15 M2 milestone report	Delivered to ROK November 2015	1.1-D
5	USA (G. Freeze)	1 - Evaluation Tools	UFDC GDSA HPC comparison report from about FY12	Delivered to ROK November 2015	1.1-E
6	ROK (S. Lee, H. Jung, G. Kim)	1 - Evaluation Tools	Updated crystalline data and parameters (granite and gneiss specifically) for PA modeling	to USA by December 2014	2.1-A
7	ROK (H. Jung)	1 - Evaluation Tools	KORAD Integrated Natural Barrier DB System (KOINS) design document	to USA by end of month December 2015	2.1-B
8	ROK (H. Jung)	1 - Evaluation Tools	Demonstration of Geo-Environmental DB for Geological Disposal KOINS	to USA at next FCAWG meeting (2016)	2.1-C
9	ROK (H. Jung)	1 - Evaluation Tools	Demonstrate structure of FEPs database being used in KOINS	to USA at next FCAWG meeting (2016)	2.1-D
10	USA (K. McMahon)	1 - Evaluation Tools	Advances in Geologic Disposal System Modeling and Application to Crystalline Rock, FCRD-UFD-2016-000440, SAND2016-9610R, September 2016	Delivered to ROK October 2016	

U.S. – Newly Available Documents re PA Modeling

#	Document Title of Deliverable
1	Mariner, P. E., E. R. Stein, J. M. Frederick, S. D. Sevougian, and G. E. Hammond 2017. *Advances in Geologic Disposal System Modeling and Shale Reference Cases*. SFWD-SFWST-2017-000044 / SAND2017-10304R. Sandia National Laboratories, Albuquerque, NM.
2	Mariner, P. E., E. R. Stein, S. D. Sevougian, L. J. Cunningham, J. M. Frederick, G. E. Hammond, T. S. Lowry, S. Jordan, and E. Basurto 2018. *Advances in Geologic Disposal Safety Assessment and an Unsaturated Alluvium Reference Case*. SFWD-SFWST-2018-000509; SAND2018-11858R. Sandia National Laboratories, Albuquerque, NM.
3	Sevougian, S. D., P. E. Mariner, L. A. Connolly, R. J. MacKinnon, R. D. Roger, D. C. Dobson, and J. L. Prouty 2019. *DOE SFWST Campaign R&D Roadmap Update*. M2SF-19SN010304042 SAND2019-5179R. Sandia National Laboratories, Albuquerque, NM.
4	Sevougian, S. D., E. R. Stein, T. LaForce, F. V. Perry, T. S. Lowry, L. J. Cunningham, M. Nole, C. B. Haukwa, K. W. Chang, and P. E. Mariner 2019. *GDSA Repository Systems Analysis Progress Report*. M2SF-19SN010304051 SAND2019-5189R. Sandia National Laboratories, Albuquerque, NM.
5	2017 and 2018 M2 milestones associated with Engineered Barrier Systems and Spent Fuel Disposition in Crystalline Rocks

Development of Safety Assessment Code for the Spent Nuclear Fuel Repository

- U.S. Tasks
  - Share documentation of U.S. safety assessment work for generic crystalline repository concepts, including assumed design information (B.3)
  - Share documentation of U.S. approaches to verification and validation (V&V) of PA models (B.1)
  - Conduct THMC modeling as part of ongoing DECOVALEX studies, share results with ROK in the context of the DECOVALEX program (B.2)

Argonne NATIONAL LABORATORY

BERKELEY LAB

Lawrence Livermore

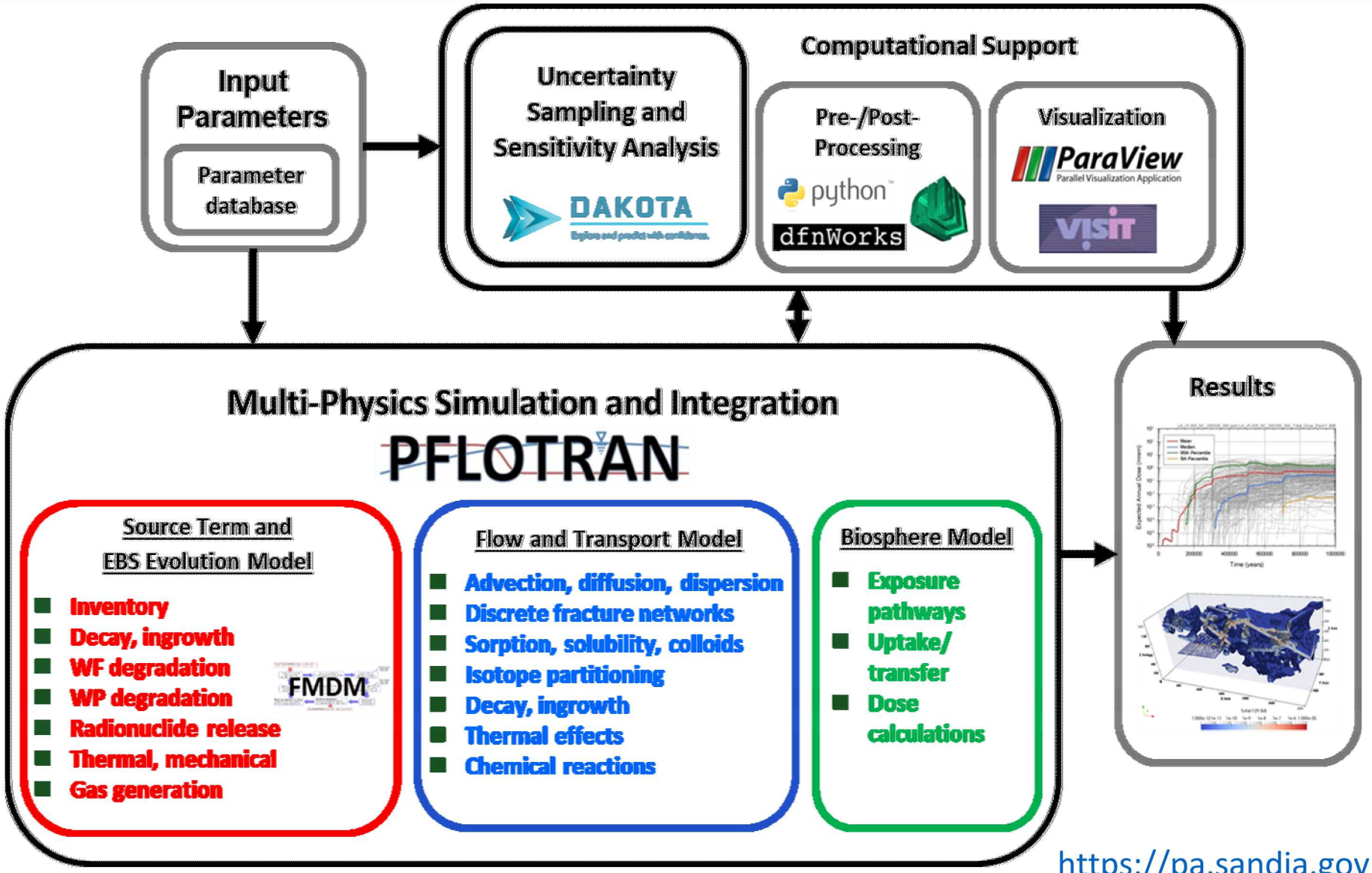
Los Alamos NATIONAL LABORATORY EST. 1943

OAK RIDGE National Laboratory

Pacific Northwest NATIONAL LABORATORY

Sandia National Laboratories

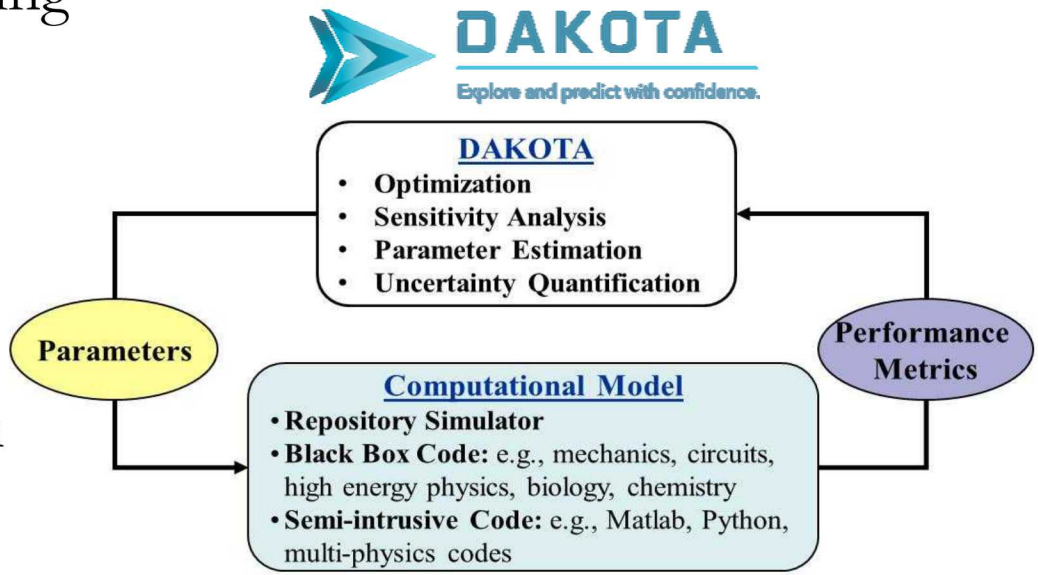
Development of Safety Assessment Code – GDSA Framework



https://pa.sandia.gov

U.S. Safety Assessment Work – Uncertainty and Sensitivity Analysis

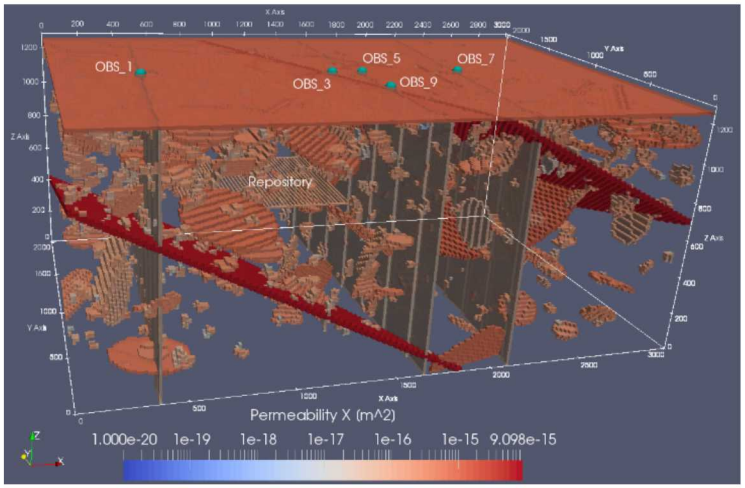
- Develop tools for uncertainty and sensitivity analysis
- Tried-and-True
  - Latin Hypercube Sampling
  - Correlation
  - Stepwise regression
  - Rank transformations
- Evolving standards
  - Variance decomposition
  - Surrogate modeling
  - Importance sampling

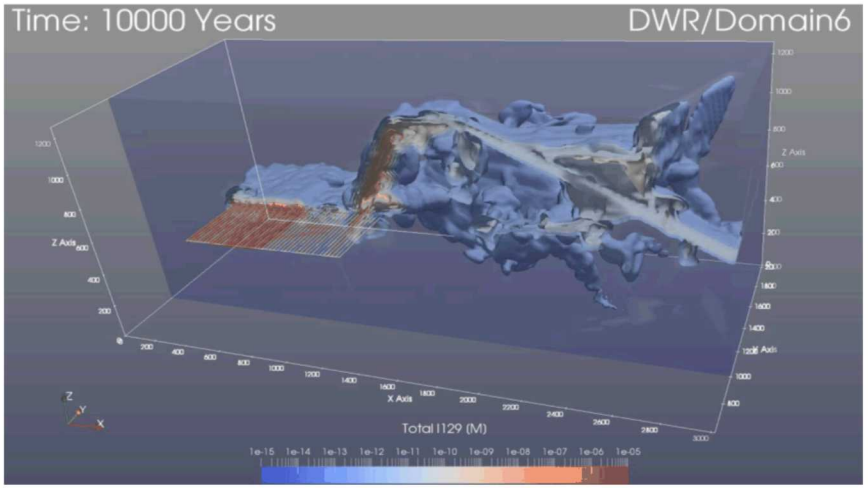


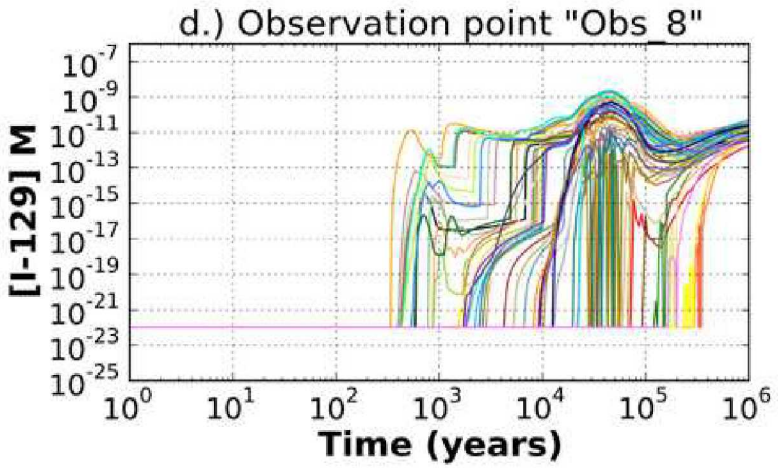
https://dakota.sandia.gov

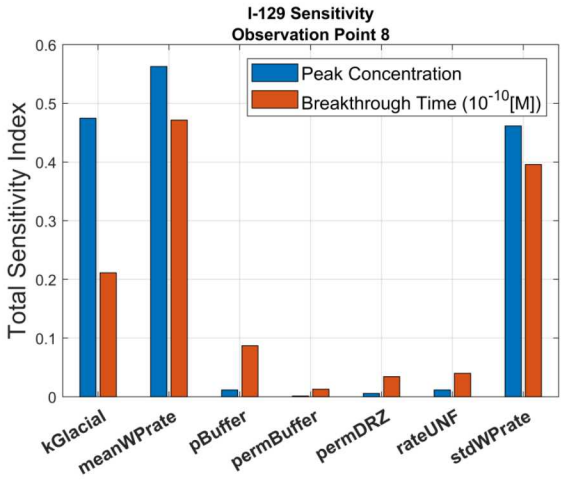
U.S. Safety Assessment Work – Crystalline Reference Case

- Expanded uncertainty and sensitivity analysis







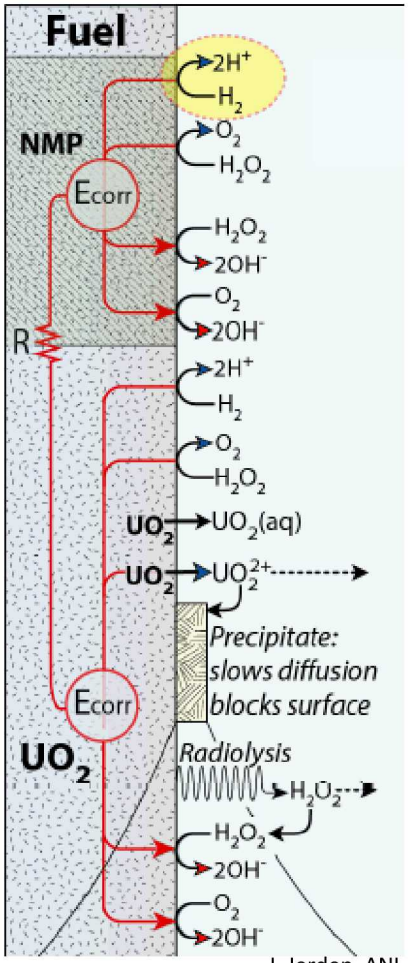


Los Alamos NATIONAL LABORATORY EST.1943

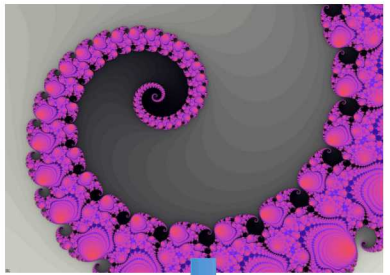
Sandia National Laboratories

U.S. Safety Assessment Work – Fuel Matrix Degradation Model (FMDM)

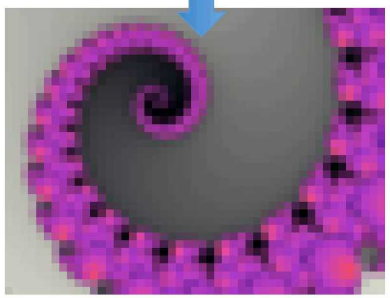
- Develop computationally efficient process model couplings



J. Jerden, ANL

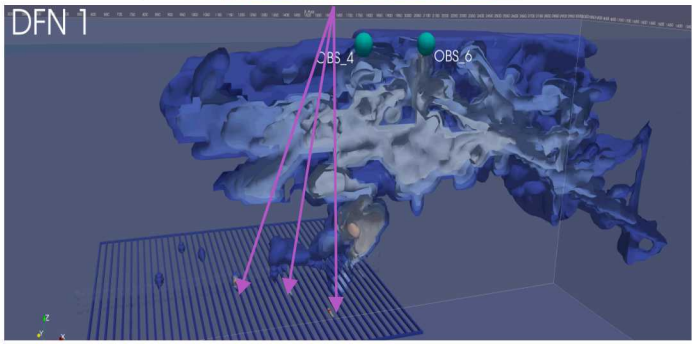


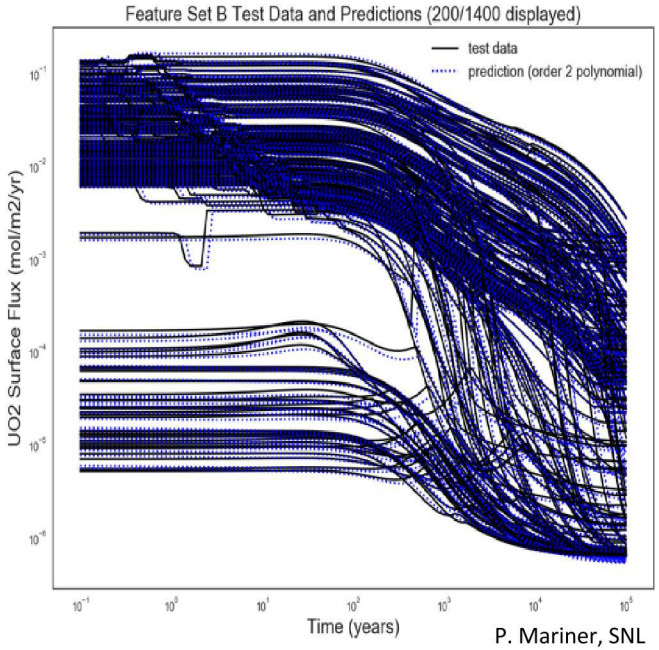
Process model



Surrogate model

PA





P. Mariner, SNL

Argonne NATIONAL LABORATORY

Sandia National Laboratories

U.S. Safety Assessment Work – Topical Areas

- Modeling flow and transport in fractured rock
  - Micro fractures and matrix diffusion (Äspö Hard Rock Laboratory)
  - Synthesis of (Mizunami) field data into flow and transport model
  - Reduced order models of fracture flow and transport
- Engineered barrier materials
  - New materials for improved stability ($Mg_3(Si, Al)_4O_{10}(OH)_2 \bullet 4H_2O$)
  - Bentonite resaturation (Äspö Hard Rock Laboratory)
- Thermochemical Database (Nuclear Energy Agency)
- Disposal of large waste packages
  - Thermal management
  - Operations (handling/emplacement)
  - Potential for criticality

Lawrence Livermore

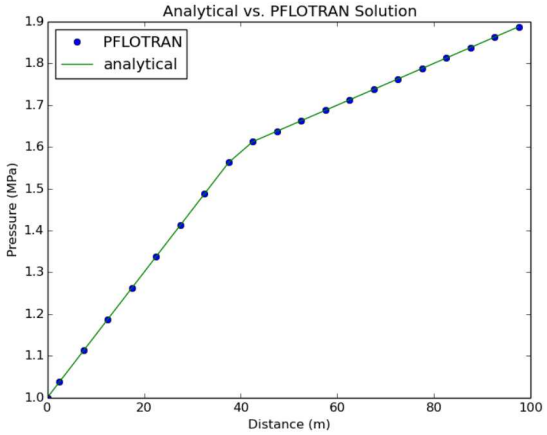
Los Alamos NATIONAL LABORATORY EST. 1943

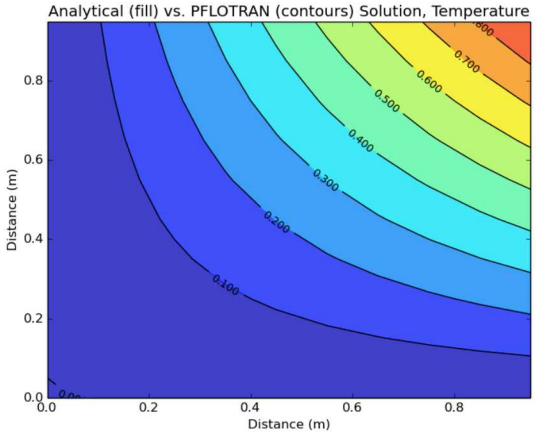
OAK RIDGE National Laboratory

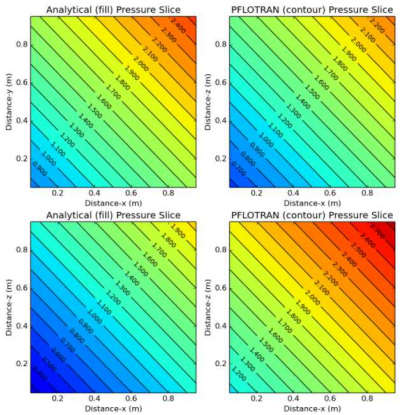
Sandia National Laboratories

U.S. Approaches to V&V – PFLOTRAN Quality Assurance (QA)

- Share documentation of U.S. approaches to verification and validation (V&V) of PA models
- QA'd release planned for 2020
- Automated QA Test Harness
  - Verification against 1-, 2-, and 3-D analytical solutions
  - Benchmark against similar codes







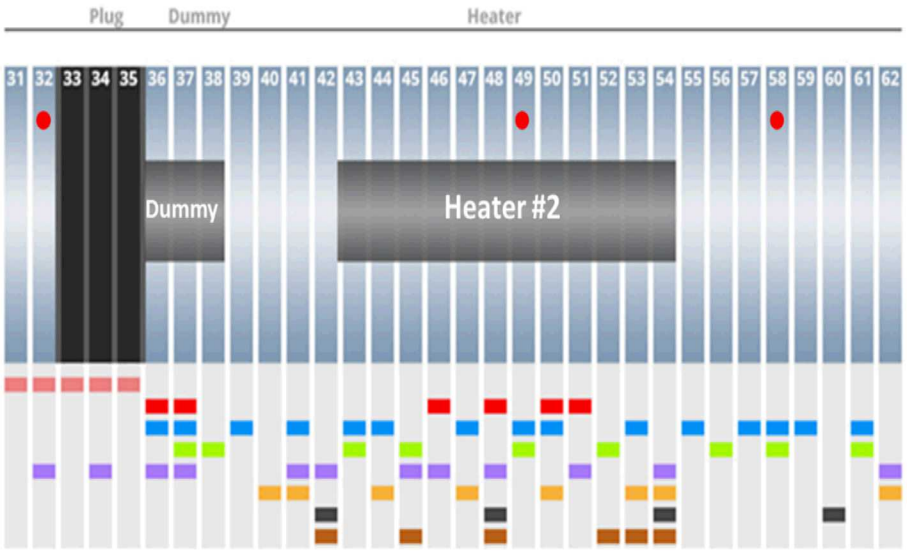
J. Frederick, SNL

https://www.pflotran.org/qa-dev/

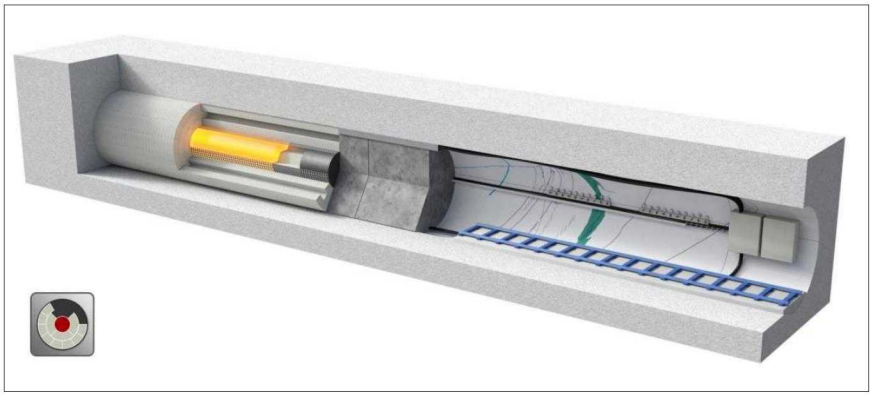
DECOVALEX - THMC MODELING

- Conduct THMC modeling as part of ongoing DECOVALEX studies, share results with ROK in the context of the DECOVALEX program

FEBEX and FEBEX-DP (100°C)



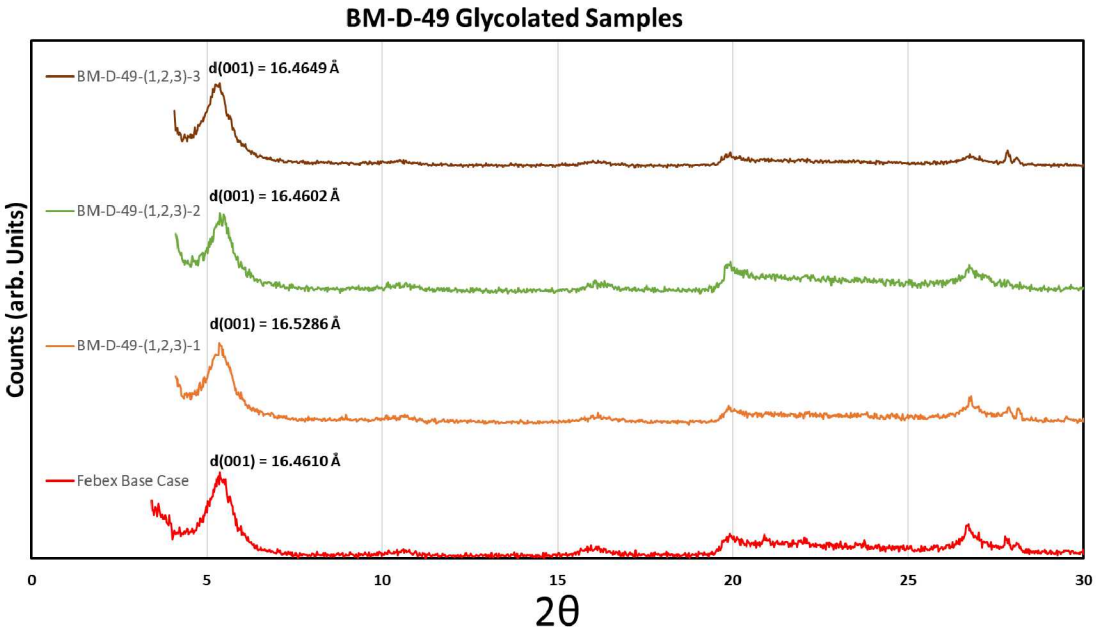
HotBENT (200°C)

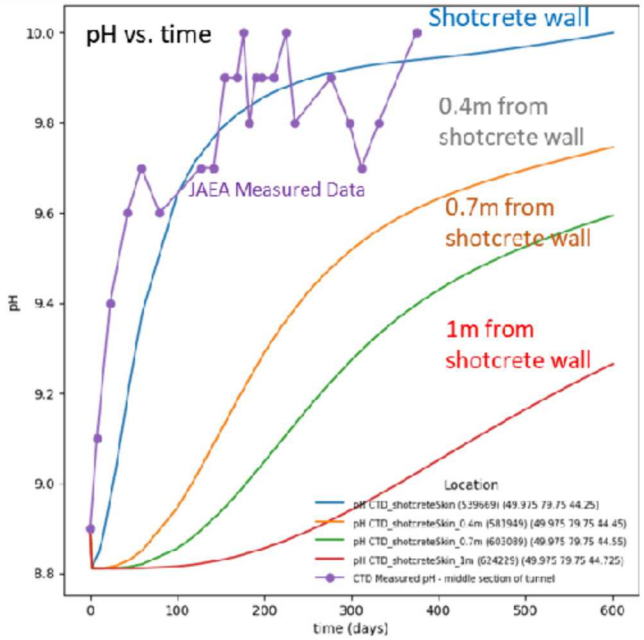


BERKELEY LAB · Los Alamos NATIONAL LABORATORY EST.1943 · Sandia National Laboratories

DECOVALEX – FEBEX AND FEBEX-DP

- Heaters operated at a maximum of 100 °C
- Samples obtained in 2015 after 18 years of heating
- THM, THC, and THMC modeling

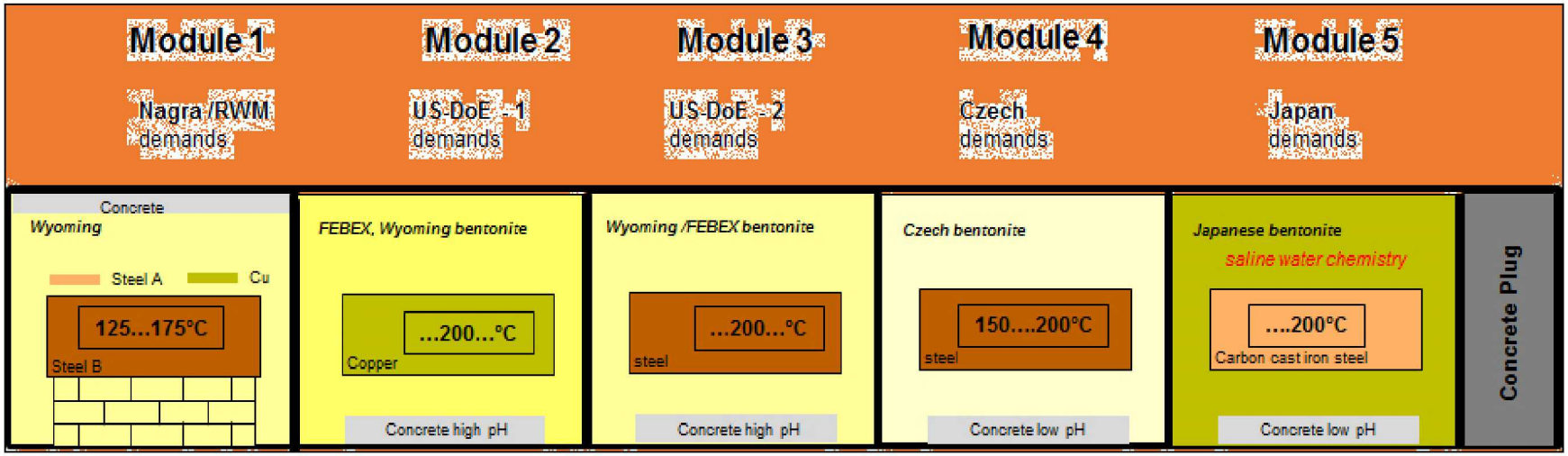




Preliminary results, Carlos Jove Colon, SNL

DECOVALEX – HOTBENT

- Heater start spring/summer 2020
- Evaluate buffer behavior at 150 °C to 200 °C
  - Cementation affecting mechanical properties
  - Illitization affecting swelling and transport
  - Thermal overpressurization and vapor convection
  - Delayed saturation and differential swelling



J. Birkholzer, LBNL

DECOVALEX 2023 – PA MODELING PROPOSAL

- Propose simulation and analysis of a generic crystalline reference case
- Conceptual model (e.g., features, processes) open to participant discussion
- Characteristics, properties, constitutive models relevant to participants
- Compare
  - Subsystem process model output
  - Deterministic reference case simulation
  - Sensitivity analysis methods
  - Probabilistic PA with propagated uncertainty