SAND2017-5233PE

Spent Fuel and Waste Science and Technology

Preview of Thursday Morning's GDSA/Process Modeling Integration Sessions

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SFWST Working Group Meeting
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Objectives

- **Background: Nov. 30 – Dec. 1, 2016 work package managers & DOE meeting in Las Vegas to discuss integration and R&D priorities**
- **Main Idea/Goal: Follow-up to Dec. meeting—Organize and coordinate (i.e., integrate) SFWST modeling activities to achieve specific system performance assessment ("GDSA Framework") *capabilities* at defined *times* (e.g., at "evaluation of candidate sites" in 20XX)**
- **Subsidiary goals include:**
  - Do current modeling/testing activities support R&D priorities in the UFD Roadmap? If not, how to adjust them?
  - Are there gaps in our process modeling, PA modeling, and/or testing activities based on UFD Roadmap priorities?
- **Method/Tool: Use GDSA/Process Model Integration Timeline as a way to establish completeness and R&D priorities**

Some "Points" to Ponder

- **Define one or two "capability points," e.g.,**
  - Near-term (2020) "complete" capability: process models and their implementation in *GDSA Framework* will have a certain "fidelity" that we start defining today
  - Farther-term (2024) "complete**r**" capability: process models and their implementation in *GDSA Framework* will have a certain higher fidelity
- **Year-by-year workscopes and activities should be designed and integrated to support either or both of these "capability points"**
- **Importance of tying back to Roadmap "Issue" (or FEP) R&D priorities?**

Working Integration Timeline to 2020

- **Discuss in detail in the 2nd Thursday morning session**
- **Green shading = known interlab integration required**

This sheet is linked to the GDSA Tasks sheet...		GDSA LOE	Fraction of task	Status/ Notes
2017				
4	SNF Degradation	M		LF = Arrhenius; no FMDM till optimized
83	Waste Form-Canister-Buffer Discretization (1D -> 3D)	M	/2	ongoing; integrate with Carlos
63	Basic biosphere model	L		mostly done
67	Numerical solution methods (analytical derivatives)	M		mostly done
62	QA, V&V (documentation and tests)	H		ongoing, partly funded by WIPP
Green shading = known interlab integration				
Blue shading = other response surfaces				

		GDSA LOE	Fraction of task	GDSA Priority	Status/ Notes
2018					
5	(Pseudo) Colloid-Facilitated Transport Model	M	/2	H	start this year
13	Simplified Representation of THMC processes in EBS (clay illitization)	M	/2	H	use GDSA reference case; LF = response surf
14	Simplified Representation of THM (BBM) model of buffer materials (unsaturated)	M	/2	H	use GDSA reference case; LF = response surf
10	Salt Coupled THM processes	H	/2	H	use GDSA reference case; LF = response surf
7	Discrete Fracture Network (DFN) Model	M - H	/3	H	real DFN w/ matrix diffusion & heat
68	Simplified Representation of Mechanical processes in PA	M		H	from Reedlunn? From WIPP, too? LF = response surf
83	Waste Form-Canister-Buffer Discretization (1D -> 3D)	M	/2	M	ongoing; integrate with Carlos
78	PFLOTRAN improvements	L		M	Checkpoint/restart capability for new process models
80	Species and element properties	L		M	temp-dependent solubilities
80	Species and element properties	L		M	Species-specific diffusivities
9	Waste Package Degradation Model (mechanistic)	L - M	/2	M	Start in 2018 for LC (include breach area)
70	Pitzer model	M - H	/2	L	Wolery version - do we have enough staff to do?

		GDSA LOE	Fraction of task	GDSA Priority	Status/ Notes
2019					
6	Intrinsic Colloids	M			combine with pseudo-colloids
5	(Pseudo) Colloid-Facilitated Transport Model	M	/2	H	finish this year
13	Simplified Representation of THMC processes in EBS (clay illitization)	M	/2	H	use GDSA reference case; LF = response surf
14	Simplified Representation of THM (BBM) model of buffer materials (unsaturated)	M	/2	H	use GDSA reference case; LF = response surf
10	Salt Coupled THM processes	H	/2	H	use GDSA reference case; LF = response surf
15	Simplified Representation of Rigid-Body-Spring-Network (RBSN)	M			DRZ fractures (not needed in Pierre shale?) LF = response surf
7	Discrete Fracture Network (DFN) Model	M - H	/3	H	real DFN w/ matrix diffusion & heat
53	In-Package Chemistry	M	/2		Jerden's work?
69	Full Representation of Chemical processes in PA	M	/2		Carlos' model? Also, HeeHo
70	Pitzer model	M - H	/2	L	Wolery version - do we have enough staff to do?
9	Waste Package Degradation Model (mechanistic)	L - M	/2	M	Start in 2018 for LC (include breach area)
73	Other missing FEPs (processes) SF-17SN01030401 SF-17SN01050402	M - H	/2		Funding dependent

2020	
7	Discrete Fracture Network (DFN) Model
53	In-Package Chemistry
52	In-Package Flow
69	Full Representation of Chemical processes in PA
51	Cladding Degradation
73	Other missing FEPs (processes) SF-17SN01030401 SF-17SN01050402
79	Disruptive events SF-17SN01030401 SF-17SN01050402
72	Surface processes and features
64	Grid refinement
62	QA, V&V (documentation and tests)

Agenda for Thursday Morning Integration Sessions

Session 1: 8:00 – 9:50 am

- **Intro & Objectives: Integration timeline (*Sevougian*)**
- **UFD Roadmap Priorities (*Sassani*)**
- ***GDSA Framework* as an Integration Tool (*Mariner*)**
- **Current R&D priorities and key process models:**
  - Argillite (*Jove-Colon*)
  - Crystalline (*Wang*)
  - Salt (*Kuhlman*)
  - International (*Zheng/Birkholzer*)
  - Deep Borehole (*Freeze*)

Session 2: 10:00 – 11:45 am

- **Integration and planning discussion (*All*)**
  - Modify integration timeline as appropriate—two approximate endpoints, 2020 & 2024
  - Discuss potential R&D modifications (or new focus) for FY18 & FY19 workscopes, to support a complete GDSA/PA capability for multiple concepts by ~2020