GDSA DPC Criticality Modeling

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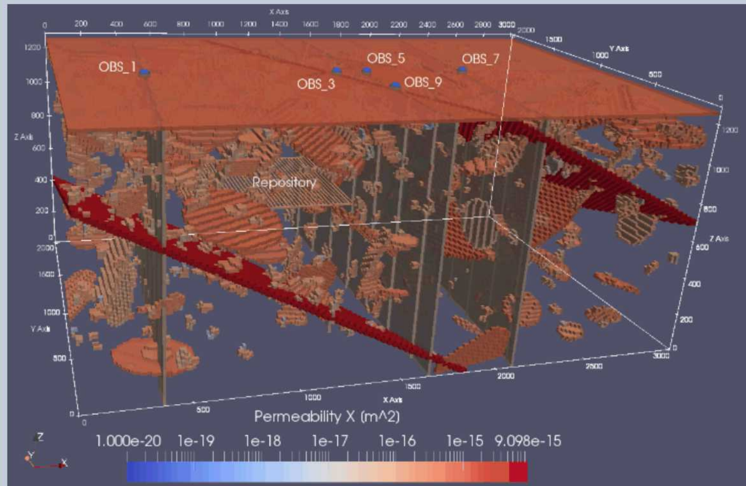

SFWD

Spent Fuel & Waste Disposition

Annual Working Group Meeting

UNLV-SEB – *Las Vegas, Nevada*

May 21-23, 2019

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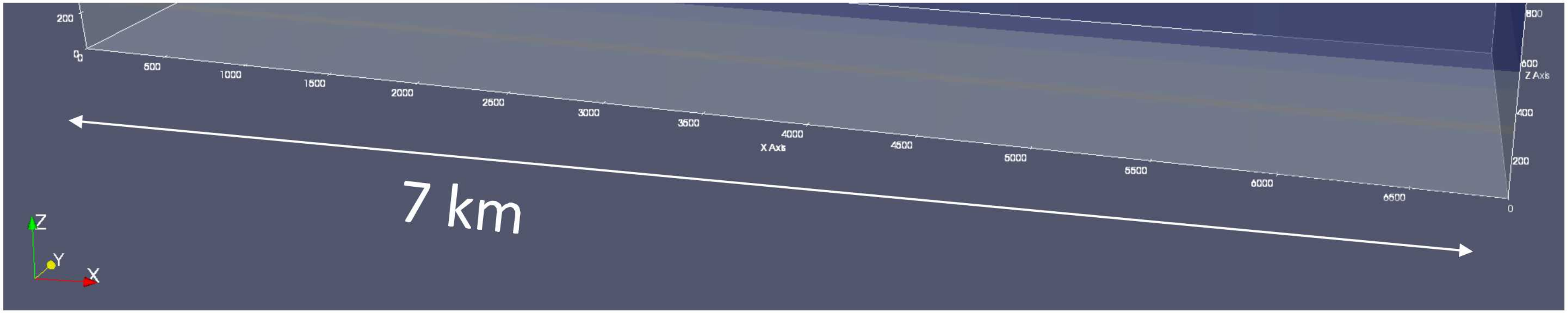
Goals

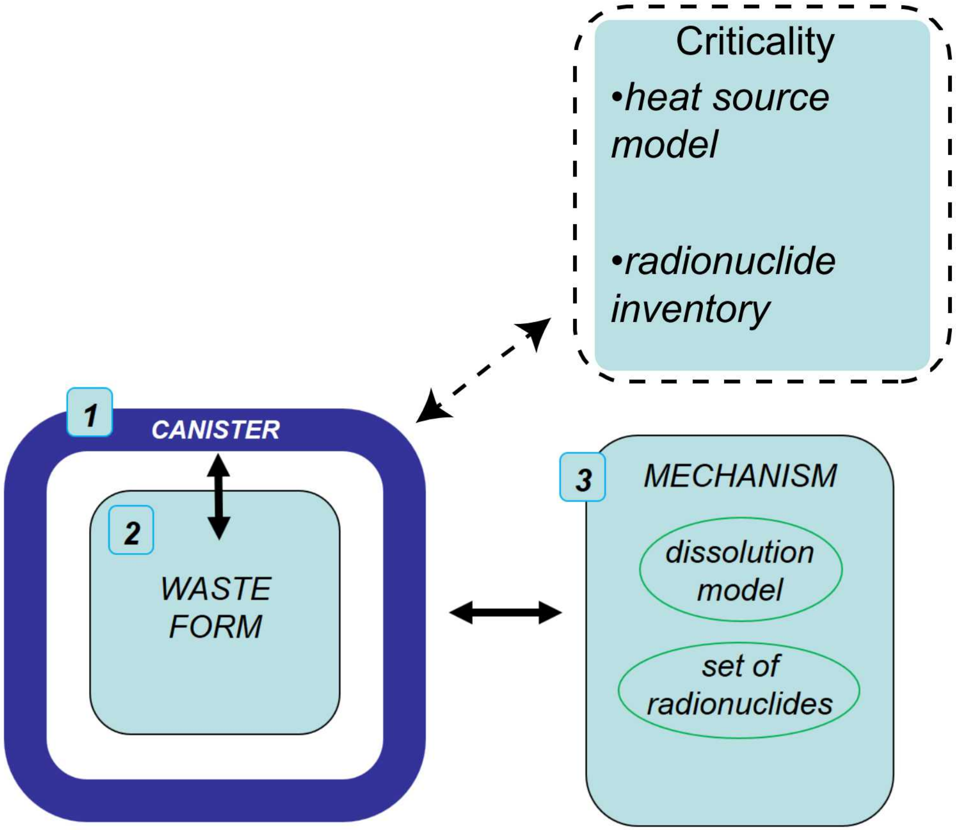
- Develop a model to study the impacts of an in-package criticality on the transport of radionuclides at scales important to PA
- Link subsurface flow and reactive transport processes modeled with PFLOTRAN to mechanistic neutronics calculations modeling local effects of a criticality on e.g. heat generation and radionuclide inventory
- Assess criticality consequences in unsaturated and saturated repositories

GDSA

- What are the potential consequences of an in-package criticality at the PA-scale?



Criticality Module



- The criticality module is built off of the waste form process model in PFLOTRAN
- Criticality parameters can be applied to any or all waste forms
- Radionuclide inventories can be read in as they evolve due to a criticality event
- Heat of criticality can be added onto decay heat

Criticality Module

```
WASTE_FORM
  COORDINATE 375.d0 0.5d0 0.5d0
  EXPOSURE_FACTOR 1.0d0
  VOLUME 2.113d0 m^3
  MECHANISM_NAME pwr_60GWdMTU
  CANISTER_BREACH_TIME 9.d3 y

  CRITICALITY
    MECH_NAME ss_criticality
    CRIT_START 9.d3
    CRIT_END 20.d4
  /
/
```

- In this example, criticality starts at 9000 years and stops at 20,000 years
- Canister breach is set to be concurrent with the start of the criticality

CRITICALITY MODULE

```
CRITICALITY_MECH
  NAME ss_criticality
  HEAT_OF_CRITICALITY 2.1d-3 #MW
  DECAY_HEAT TOTAL
    DATASET ./decay_heat_ornl_1118.ext
  /
  INVENTORY
    DATASET ./rad_inventory.ext
  /
/
```

- Heat of the criticality event is specified
- Decay heat can be read in from an external file as:
  - Total: total decay heat including criticality
  - Additional: decay heat due only to criticality
- Radionuclide inventory is read in from an external dataset as a function of time

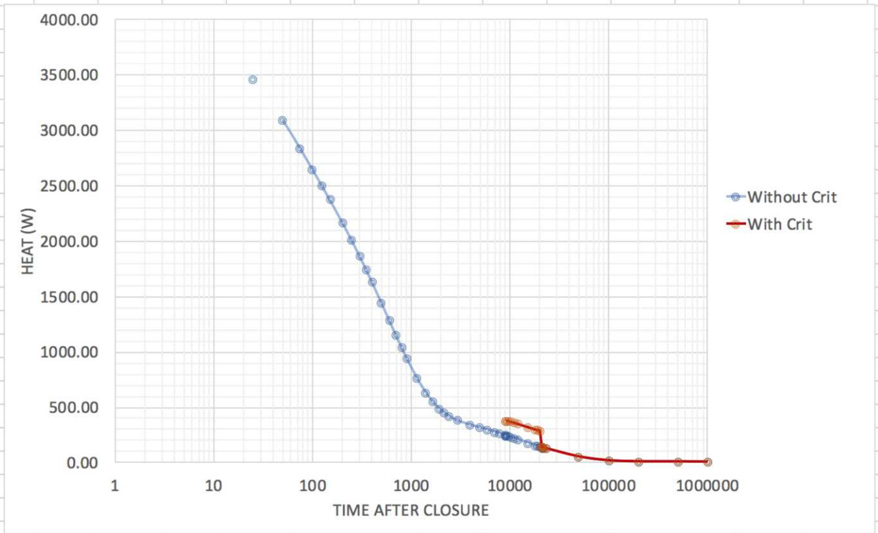
CRITICALITY MODULE

```
CRITICALITY_MECH
  NAME ss_criticality
  HEAT_OF_CRITICALITY 2.1d-3 #MW
  DECAY_HEAT TOTAL
    DATASET ./decay_heat_ornl_1118.ext
  /
  INVENTORY
    DATASET ./rad_inventory.ext
  /
/
```

- In this model, total decay heat is read in
- Heat of criticality is added during the criticality event

Time after closure (Yr)	Decay Heat Without Criticality (W)	Decay Heat with Criticality – Criticality stops at 20000 (W)	Diff
0	4002.73		-4002.73
25	3459.25		-3459.25
50	3097.82		-3097.82
75	2843.38		-2843.38
100	2653.15		-2653.15
125	2502.66		-2502.66
150	2377.76		-2377.76
200	2174.78		-2174.78
250	2009.67		-2009.67
300	1868.45		-1868.45
350	1744.46		-1744.46
400	1633.90		-1633.90
500	1444.05		-1444.05
600	1286.46		-1286.46
700	1153.87		-1153.87
800	1041.46		-1041.46
900	945.72		-945.72
1150	762.89		-762.89
1400	638.45		-638.45
1650	552.99		-552.99
1900	493.68		-493.68
2150	451.92		-451.92
2400	421.97		-421.97
2900	383.32		-383.32
3900	343.34		-343.34
4900	319.02		-319.02
5900	299.20		-299.20
6900	281.51		-281.51

Note: Criticality starts at 9000 years after closure



CRITICALITY MODULE

```
CRITICALITY_MECH
  NAME ss_criticality
  HEAT_OF_CRITICALITY 2.1d-3 #MW
  DECAY_HEAT TOTAL
    DATASET ./decay_heat_ornl_1118.ext
  /
  INVENTORY
    DATASET ./rad_inventory.ext
  /
/
```

- Radionuclide inventories are read in as a function of time

```
Total (37 assemblies) Nuclide concentrations in grams

ac227    0.00100049
ag109    1099.8199999999997
am241    3.24803
am242    3.637000000000001e-08
am243    532.111
ba137m   1.3408599999999997e-07
c14    0.4115730000000001
ce144    0.025359600000000003
cl36   3.7612299999999996e-25
cm242    7.3454999999999985e-06
cm244    0.017178199999999994
cm245    9.20272
cs133    15488.3
cs134    0.0160871
cs135    6324.100000000001
cs137    0.87549
eu151    202.10399999999996
eu153    1541.0700000000002
eu154    0.0352258
gd155    101.41699999999997
i129   2112.2000000000003
mo95   10575.600000000002
nd143    11530.999999999998
nd145    9037.999999999998
np237    28460.4
pa231    1.5151900000000003
pb210    0.023679399999999996
pm147    0.04051369999999999
pr144    1.06819e-06
pu238    1.3530499999999996
pu239    78512.0
pu240    12739.600000000002
```

Toy Problem Description

Saturated System

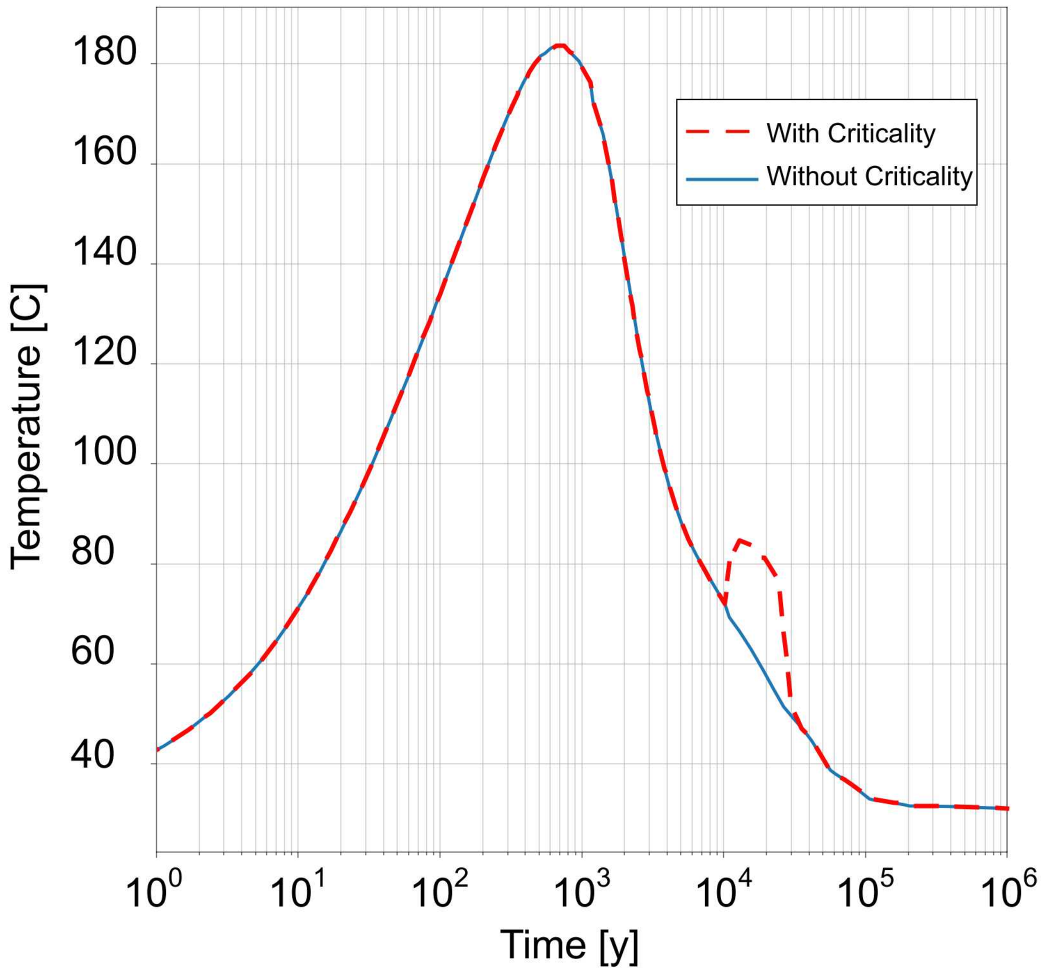
- Simple 1D, homogeneous medium with one 37-PWR waste form in the center
- Porosity: 25%
- Permeability: 1x10^{-15} m^2
- Initial Pressure: 5 MPa
- Initial Temperature: 80 C
- Initial water saturation: 100%

Unsaturated System

- Simple 1D, homogeneous medium with one 37-PWR waste form in the center
- Porosity: 25%
- Permeability: 1x10^{-15} m^2
- Initial Pressure: 5 MPa
- Initial Temperature: 80 C
- Initial water saturation: 40%

RESULTS

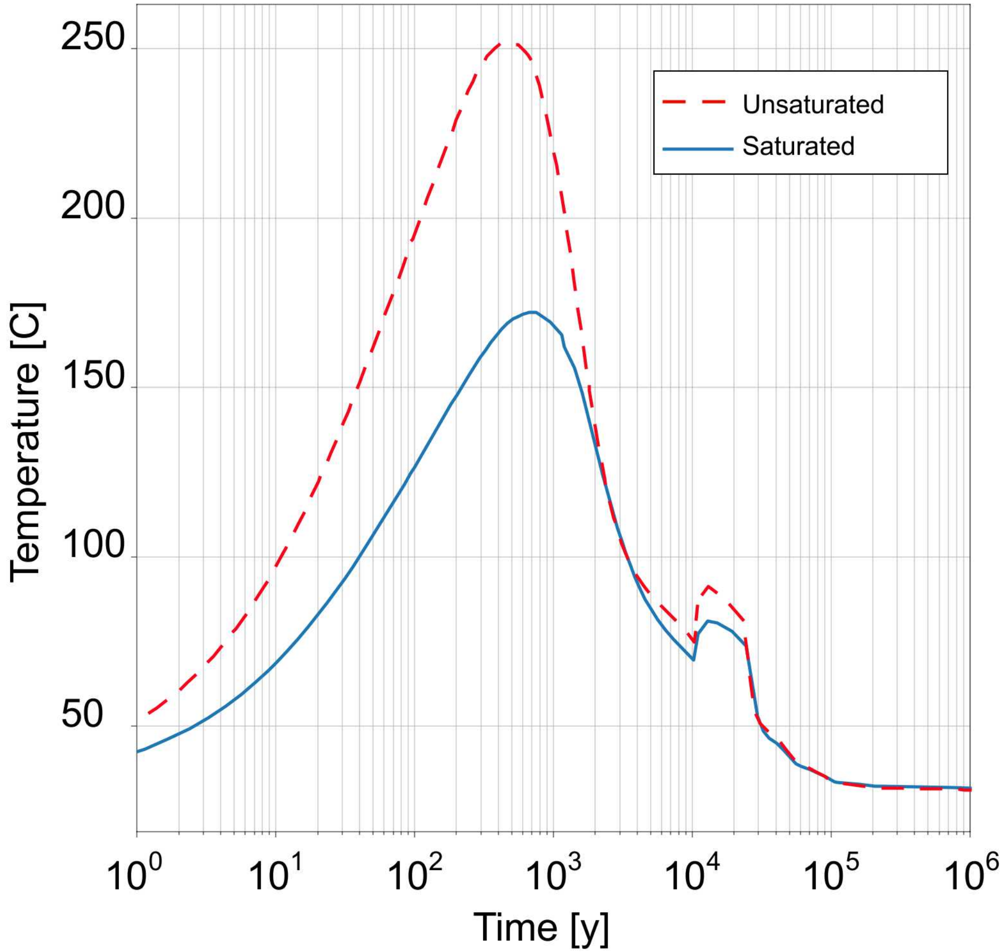
Temperature at the Waste Package, Saturated Case



- Criticality event increases temperature at the waste package by ~15 C
- Criticality event occurs after the peak temperature near the waste form

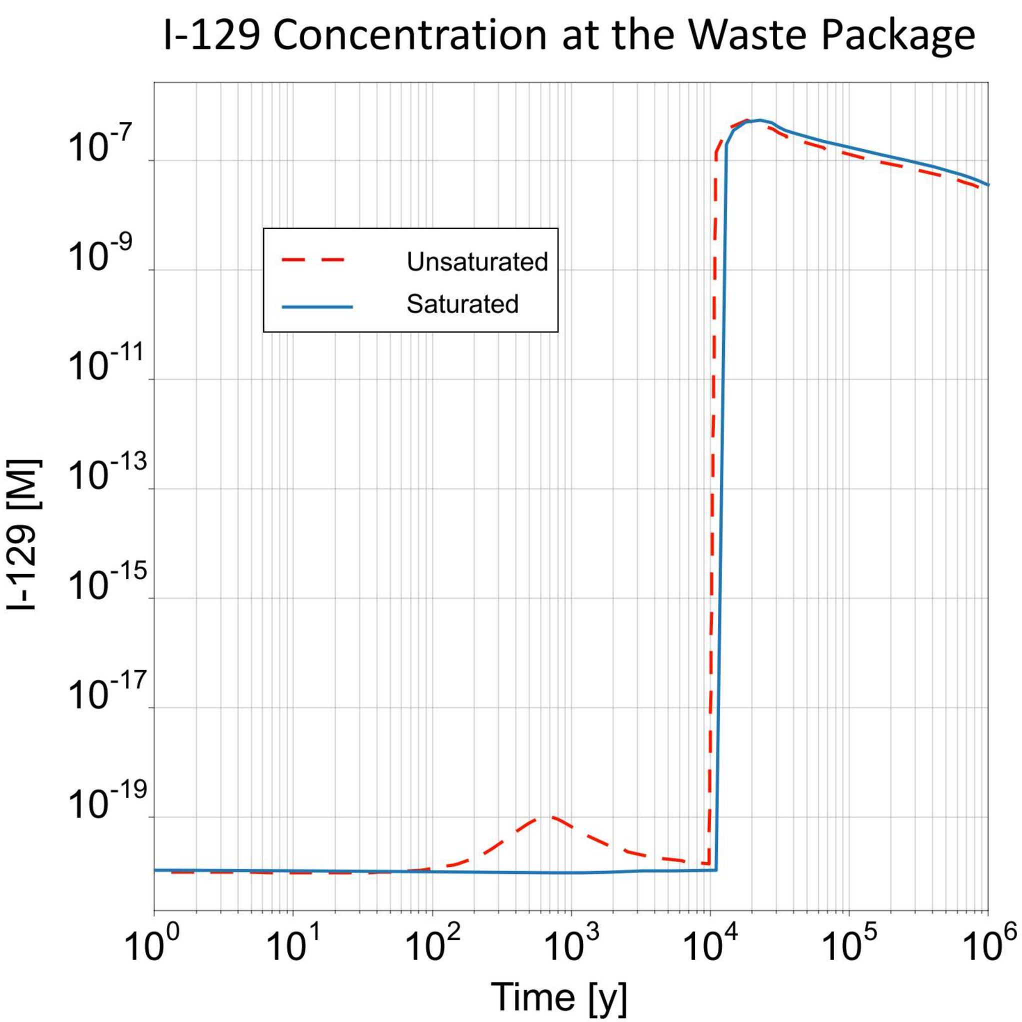
Results

Temperature at the Waste Package



- Waste package temperature in the unsaturated system can get much higher than the fully saturated case
- Similarly, the heat of criticality increases temperature more in the unsaturated case than the saturated case

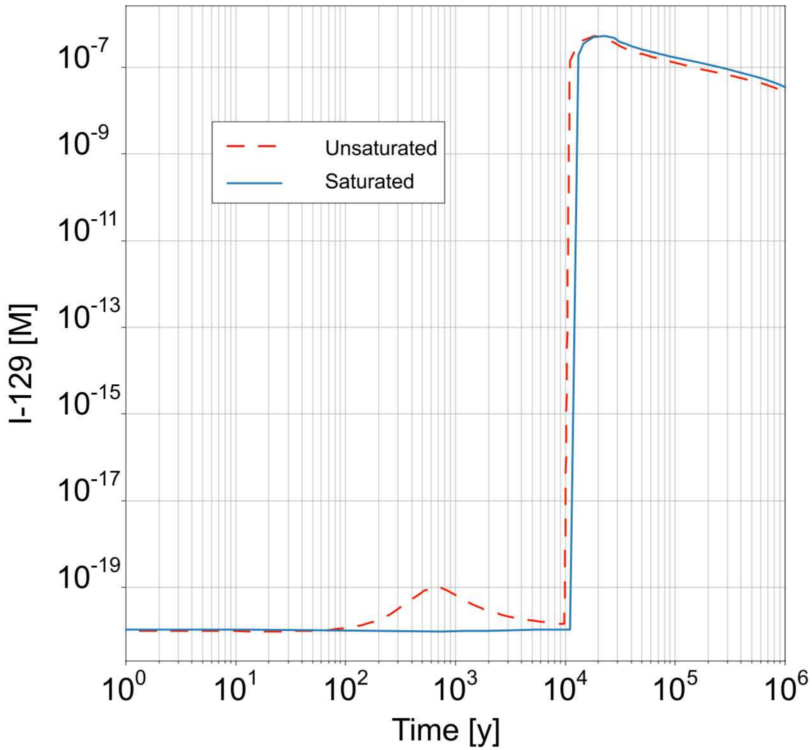
RESULTS

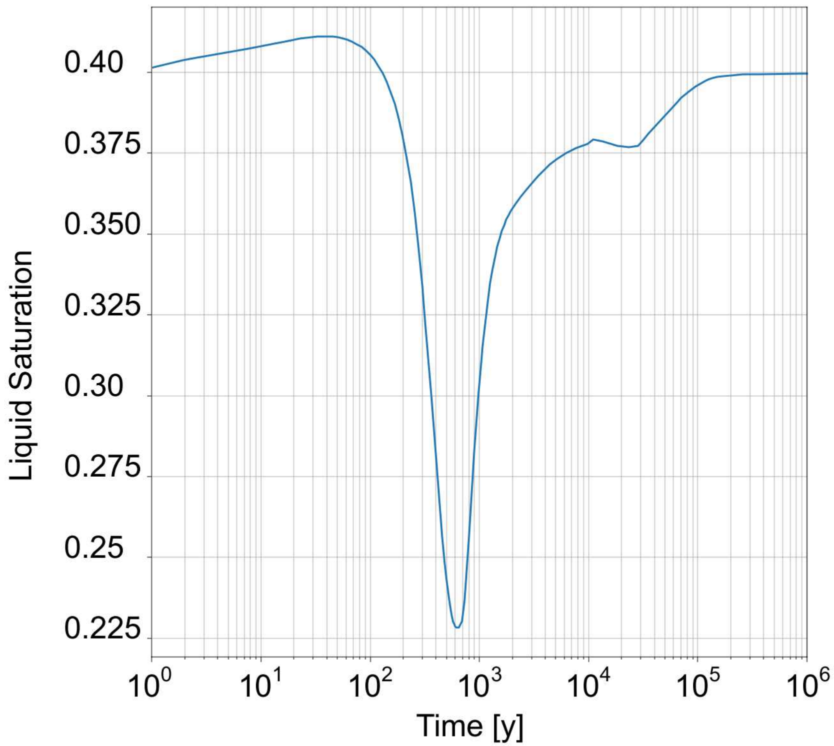


- I-129 concentrations are insensitive to the criticality when it is concurrent with waste package breach and after peak temperature

RESULTS

- I-129 concentration increases by an order of magnitude when liquid saturation reaches a minimum, which is concurrent with peak waste package temperature





CONCLUSIONS

- We are developing a module for examining consequences of in-package criticality in a DPC
- Thermal loading due to a criticality event can be applied independently to each waste form and heat output can be read in from external files
- Radionuclide inventories can also be read in from external files to capture physics of a criticality event not currently included in PFLOTRAN

Questions?

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