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Modeling and Simulation Results for Aluminum-clad SNF in DOE Sealed Standard Canisters

NWTRB Summer Board Meeting

Idaho National Laboratory

Overview

- Improve prior engineering assumptions for DOE sealed standard canisters (DOE-REP-104[1])
  - Hydrogen content and total pressure (flammability and canister failure concerns)
  - Aluminum-clad spent nuclear fuel (ASNF)
  - Modeled fuel storage of advanced test reactor (ATR), Missouri University Research Reactor (MURR), High Flux Isotope Reactor (HFIR)

- Improve with 3D computational fluid dynamics (CFD) modeling
  - 720 CPUs on INL's Falcon supercomputer
  - Star-CCM+ CFD used for fully resolved temperature data
  - 50 year timeframe requires multiscale time-stepping
  - Coupled with Cantera chemistry package for gas phase chemistry and surface chemistry

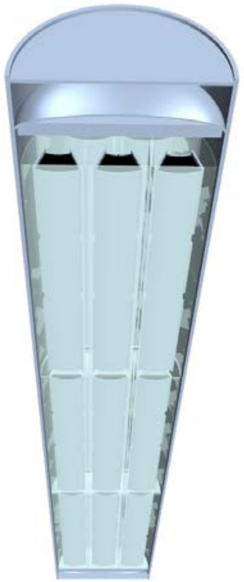
- Work has been independently reviewed by Pacific Northwest National Laboratory
  - No modifications to methodology needed
  - Clarification made in reports

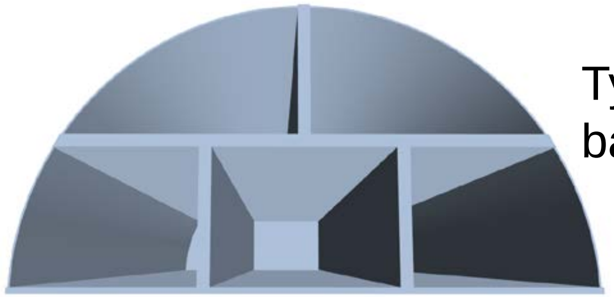
[1]Wertsching, A.K., Hill, T.J., Mackay, N. and Birk, S.M., 2007. Material Interactions on Canister Integrity During Storage and Transport. Tech. rep. Idaho National Laboratory, DOE/SNF/REP-104.

DOE Sealed Standard Canister

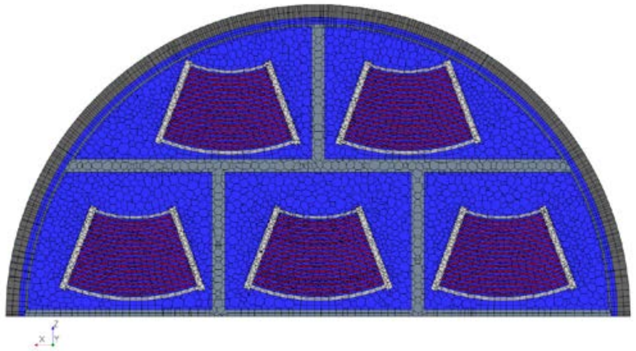
- ATR fuel expected to be loaded in 18” Diameter canister, 15-foot height with 3 Type-1a buckets loaded with 10 ATR elements each
- Symmetry condition used in thermal model

DOE Canister

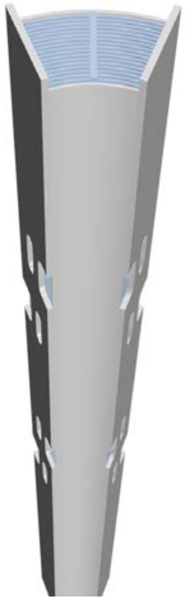




Type-1a basket



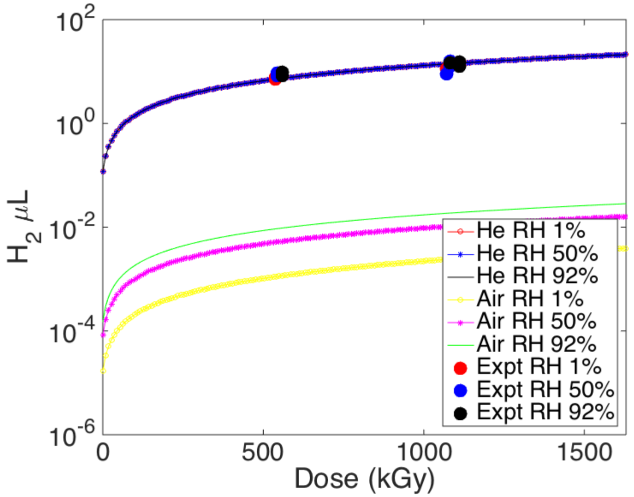
ATR



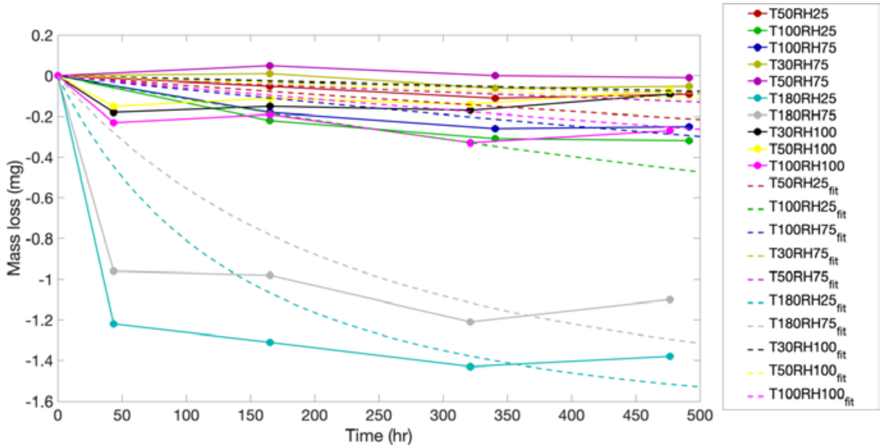
Chemistry Model

- Gas phase utilizes Wittman & Hansen model 40 species 110+ equations coupled with surface chemistry
  - Goal to model H_2 and total pressure accurately
- Three solid chemistry equations
  - Using updated G-values (H_2 radiolysis generation) from previous Task 2 presentation for helium environment
    - 2.92 - 4.12 x 10^{-4} µmol H_2/J (RH% 50-0)
  - Fit mass loss data from Task 1 to thermal dehydration of pseudo-boehmite (water absorption in corrosion layer can vary)
    - Generates water vapor, can increase pressure and contribute to H_2 generation
  - Use general corrosion rate of aluminum in water from Argonne National Laboratory (ANL) report (Hilton 2000)
    - Small H_2 generation
- Validation of chemistry model occurs over range of RH and Temperature compared to Task 1/2 results

Validation of Task 2 data w/model



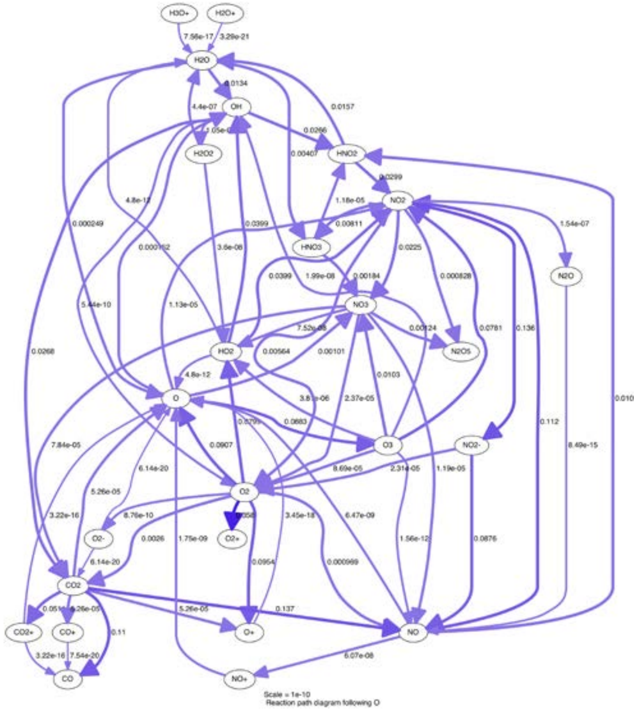
Validation of Task 1 data w/model



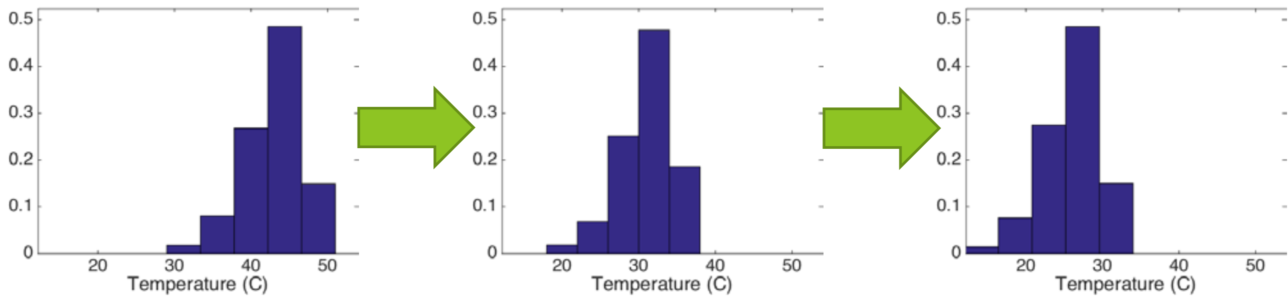
Model Chemistry Overview

- The full reaction network is too complex for reasonable simulation time
- Fully resolve 50-year thermal field in CFD model
- Use 5-environment temperature distribution to resolve chemistry in Cantera accounting for spatial temperature differences

O pathway

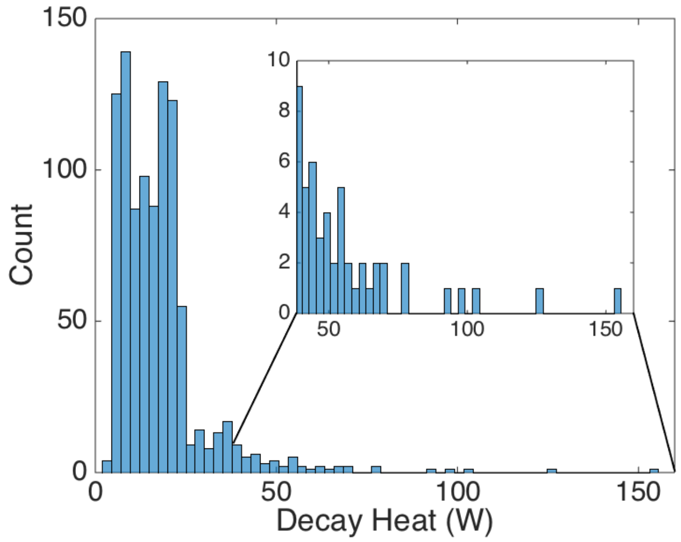


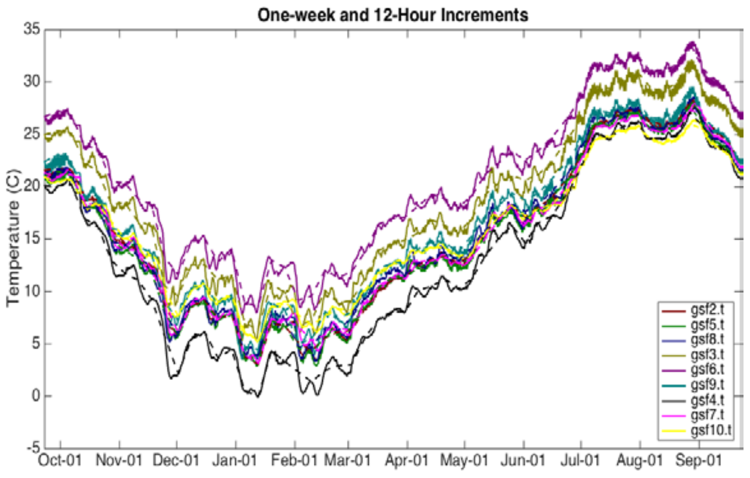
Temperature evolution



Parameter Determination

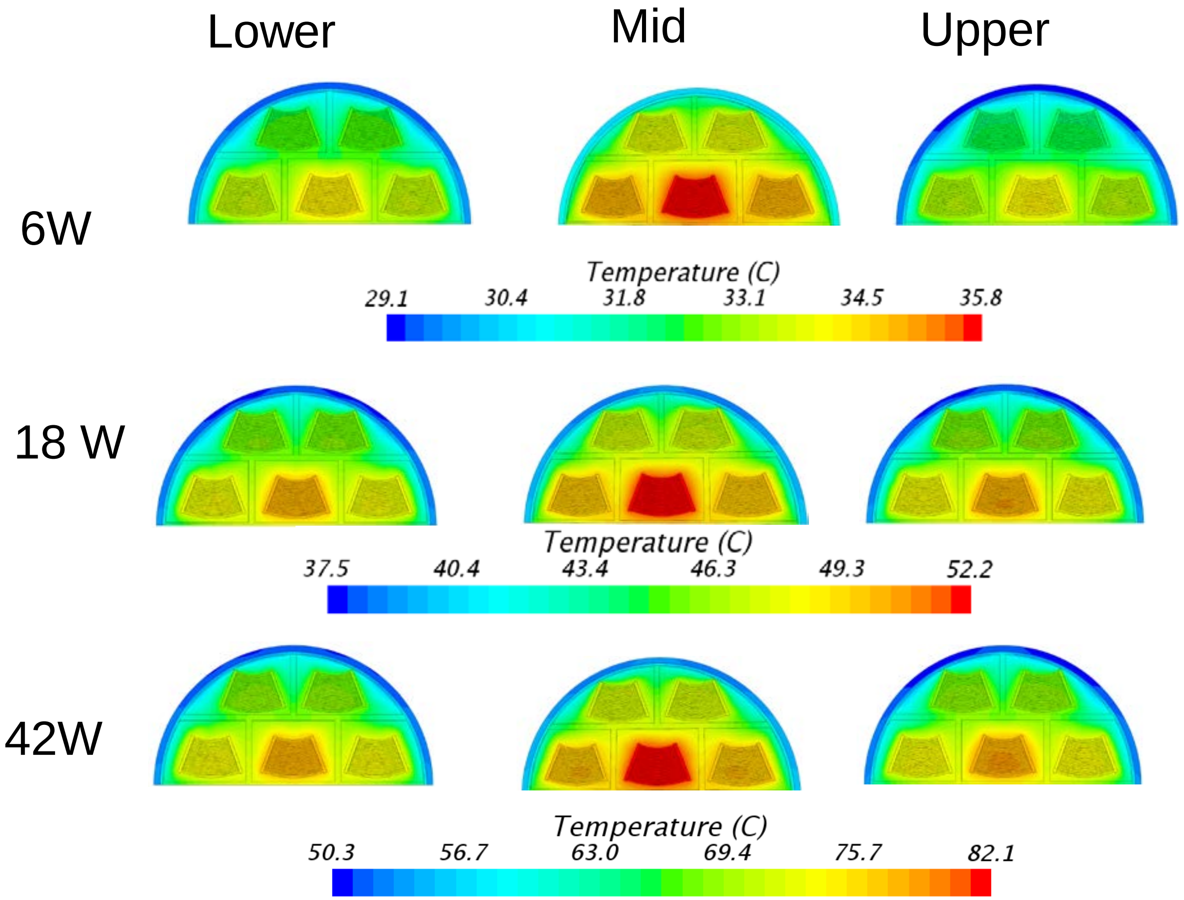
- CFD & chemical model requires set of parameters for initial condition
- Fuel decay heat
  - Inventory list: Average decay heat 18 W, with 12 W std. dev, used 1 std. dev below and 2 above
  - Decay over time w/ Cs half-life, dose rate based on decay heat
- External temperature – assumed similar to INL site history temps
  - Fluctuate with seasonal variations
- Water content
  - Residual water at 1-100% RH
- Oxide Film Thickness
  - 5 µm to 15 µm range based on MURR (Olsen et al., SRNL 2019 report) and RERTR tests (Kim et al. 2008)
  - Much lower than DOE-REP-104 assumption (34 µm)
- Additional sealed cases with 1% air contamination

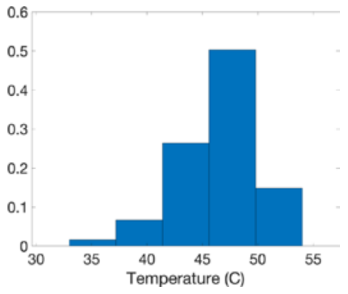


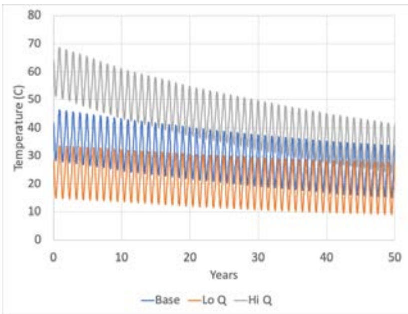


ATR Sealed Canister Velocities/Temperatures

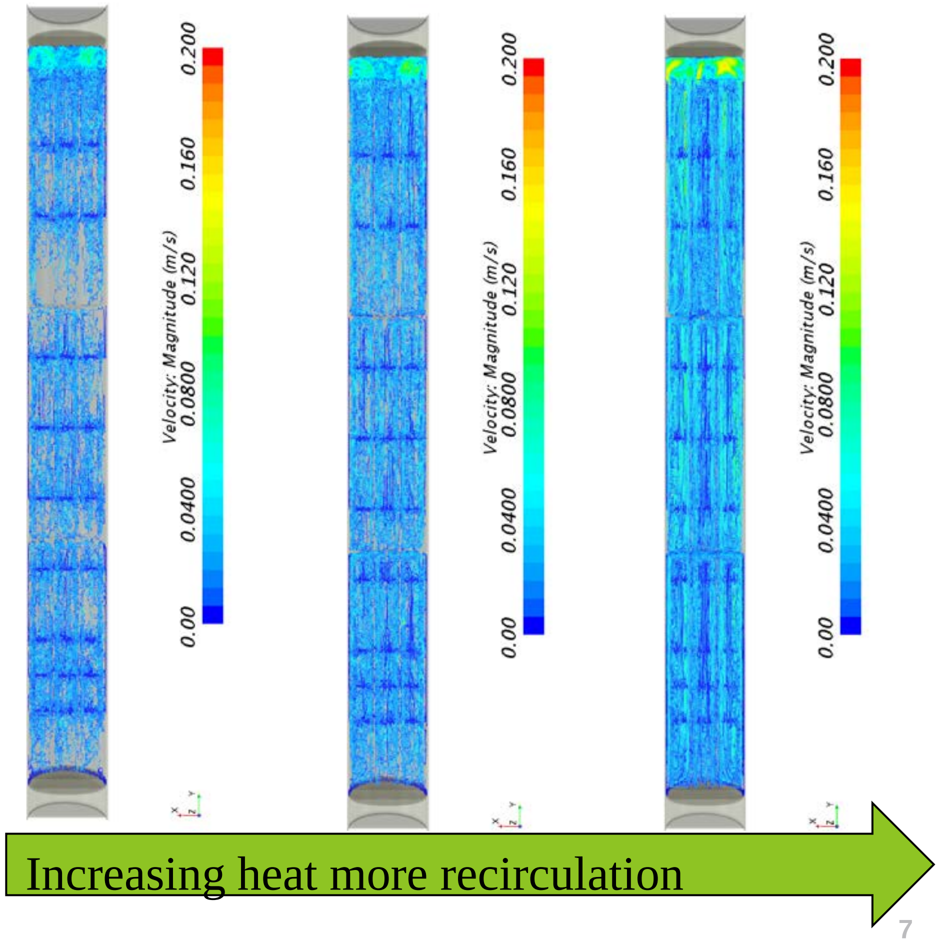
- Use CFD temperature to initialize Cantera with 5 temperature zones, and use recirculation flow as mass exchange between zones





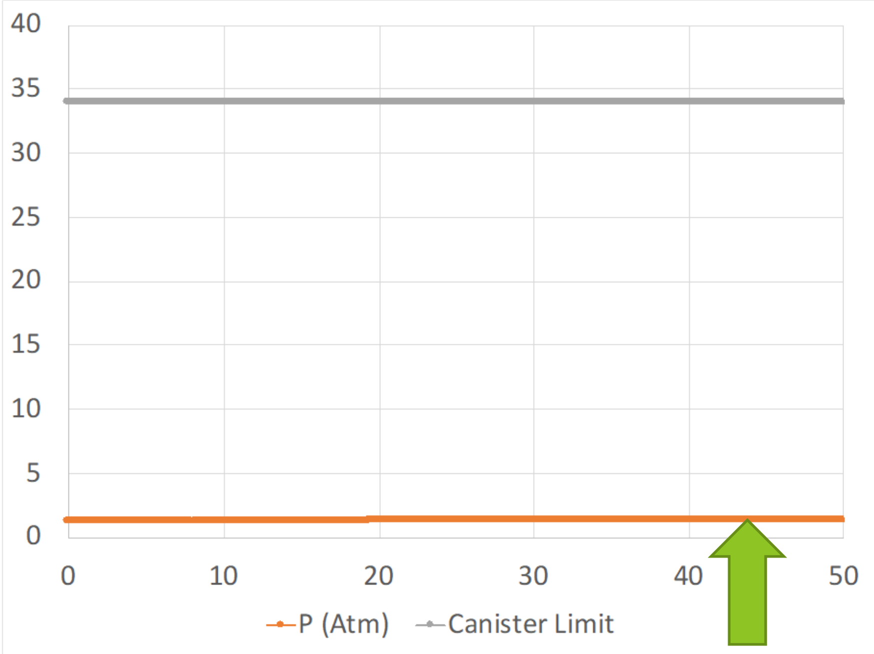


50-year thermal history

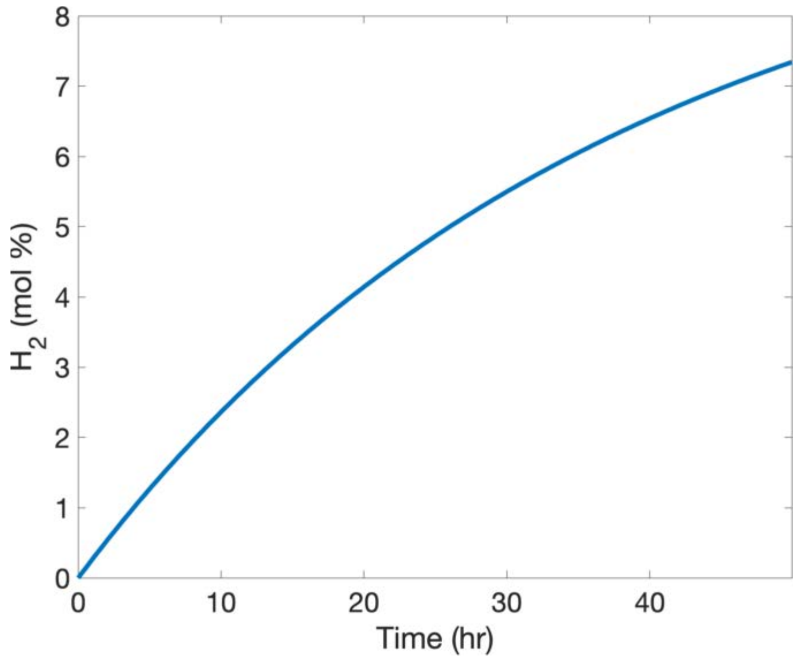


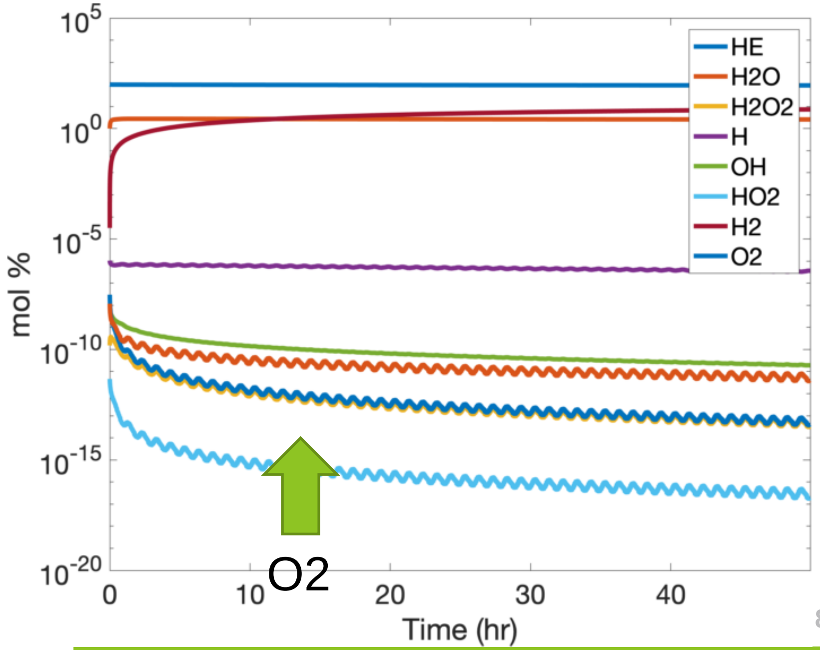
ATR DOE Standard Sealed Canister - Chemistry

- For a nominal DOE standard canister with ATR fuel (18 W decay heat, 10 µm thickness, dried 1.01:1 H_2O:Al_2O_3) in pure Helium
- Only H_2, H_2O and He significant species present (> ppm)
- 1.36 atm total pressure, 7% H_2 by year 50 of storage, no residual oxygen (<ppb) present



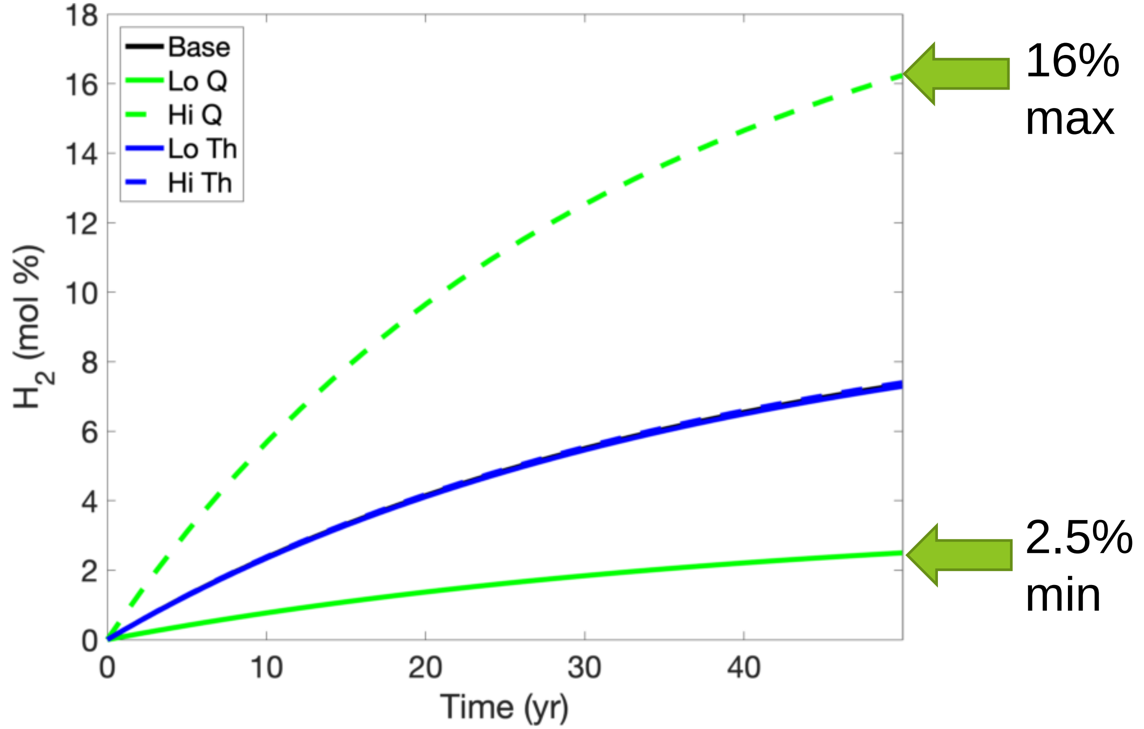
Order of magnitude
lower than canister limit

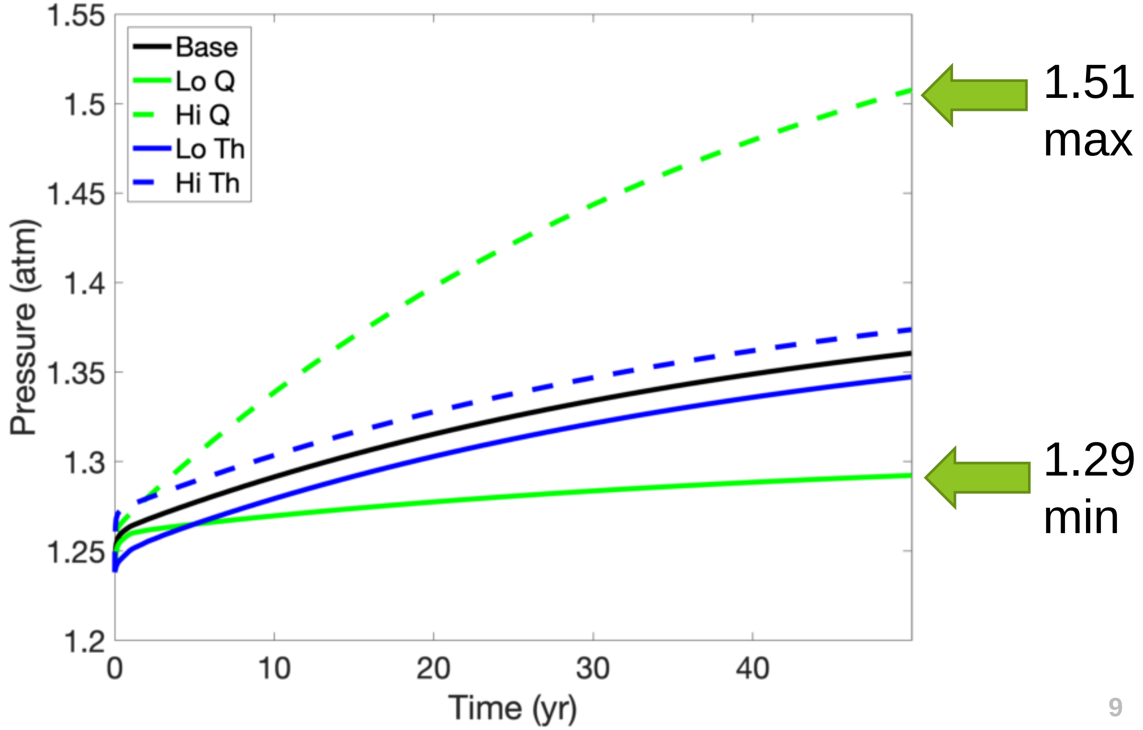




ATR DOE Standard Sealed Canister - Chemistry

- Condition changes with oxide thickness are very small
- Changes from high to low decay heat larger



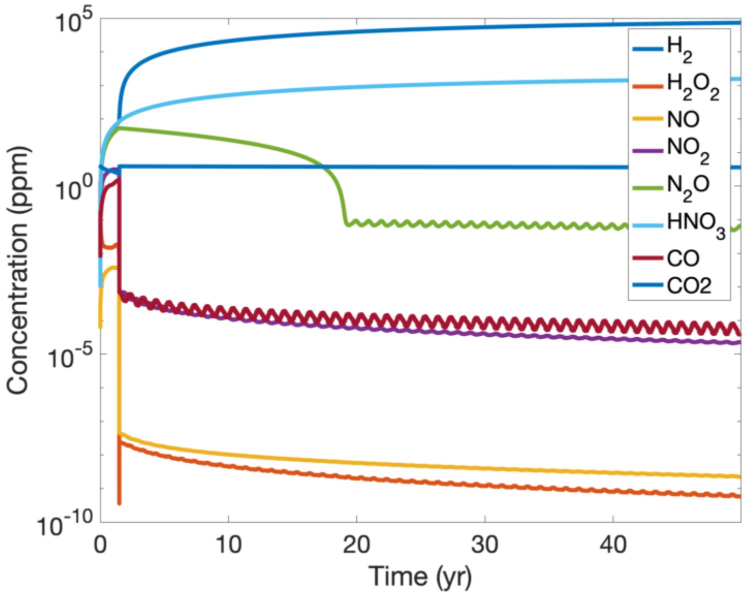


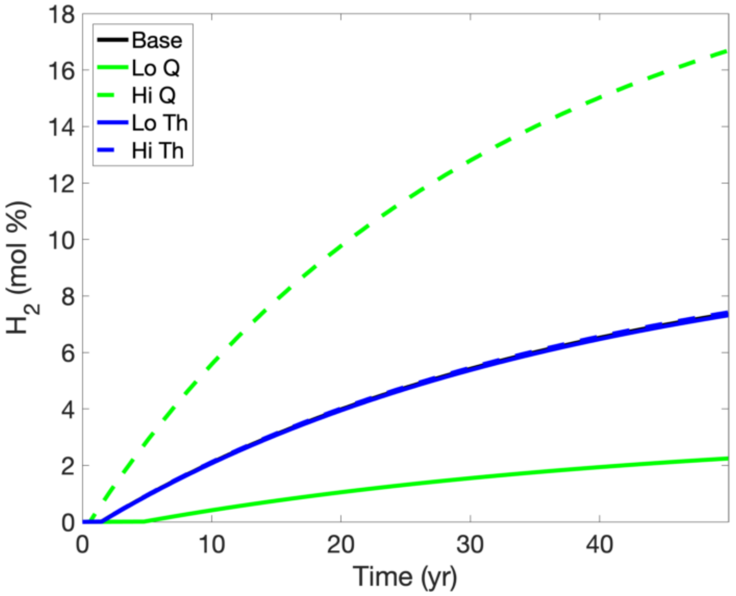
Q: Decay heat
Th: Oxide Thickness

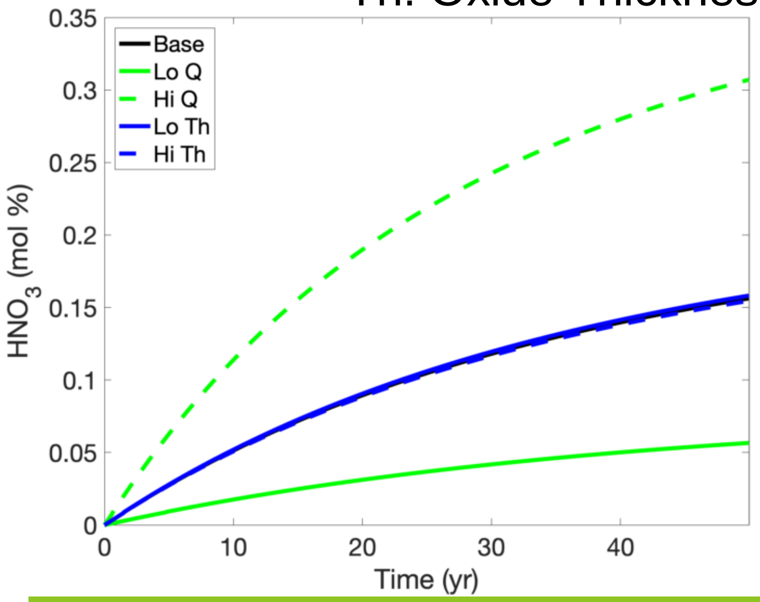
ATR DOE Standard Sealed Canister – Chemistry + 1% air

- Changes in H_2 formation and total pressure with residual air small
- HNO_3 only other major species present
- Nominally 1500 ppm HNO_3 after 50 years, max 3000 ppm with high decay heat
    - Minimal SS corrosion expected

Q: decay heat
Th: Oxide Thickness

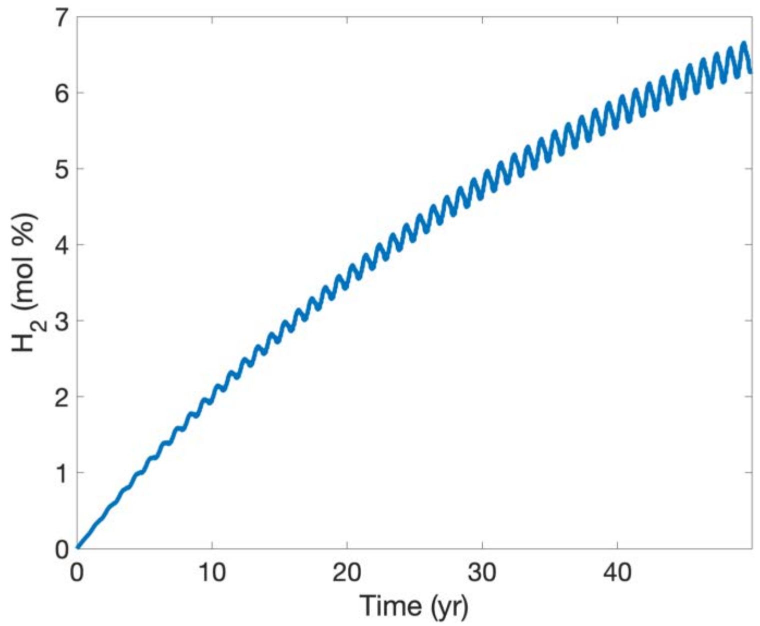


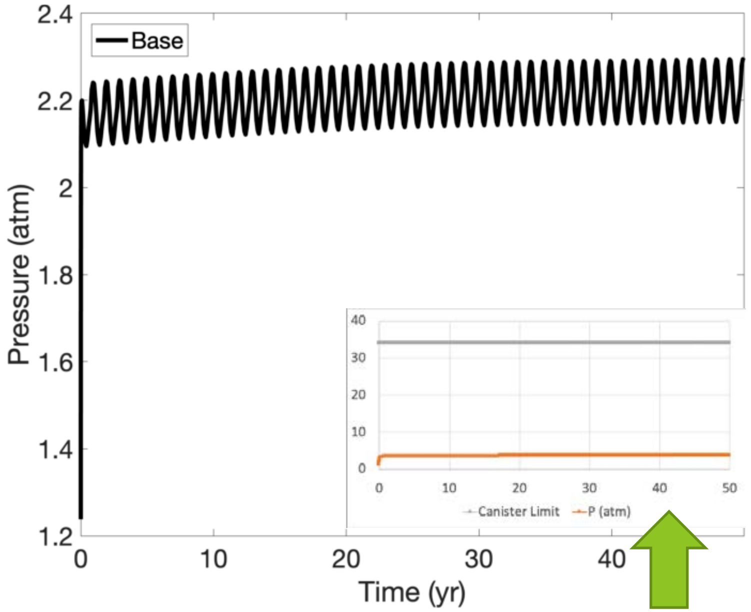


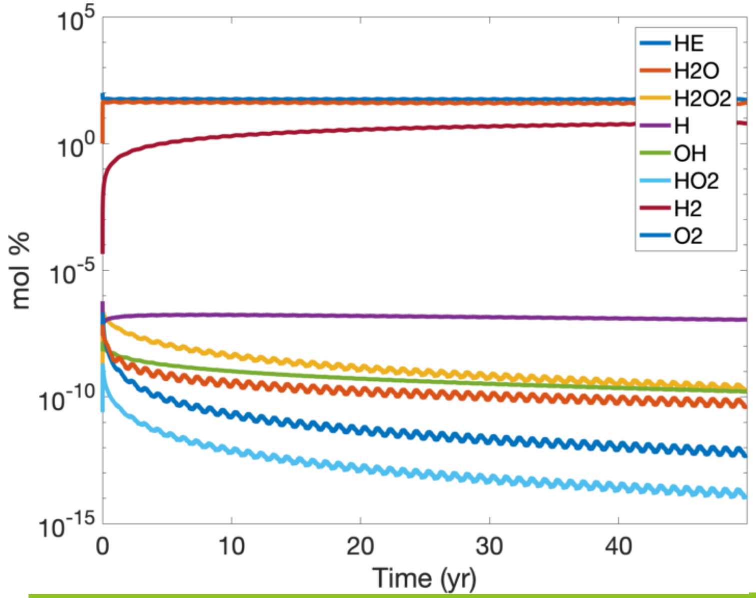


ATR Residual Pseudo-Boehmite Case

- Considered insufficient drying 2.5:1 $H_2O:Al_2O_3$ (fully saturated) on surface corrosion layer
- Thermal dehydration + residual water present, increases to 2.3 atm total pressure (from 1.36)
- Initial water release increases pressure,
  - no other species (H_2O_2/OH) present in large quantities,
  - negligible increase in H_2 from fully dried scenario, negligible O_2



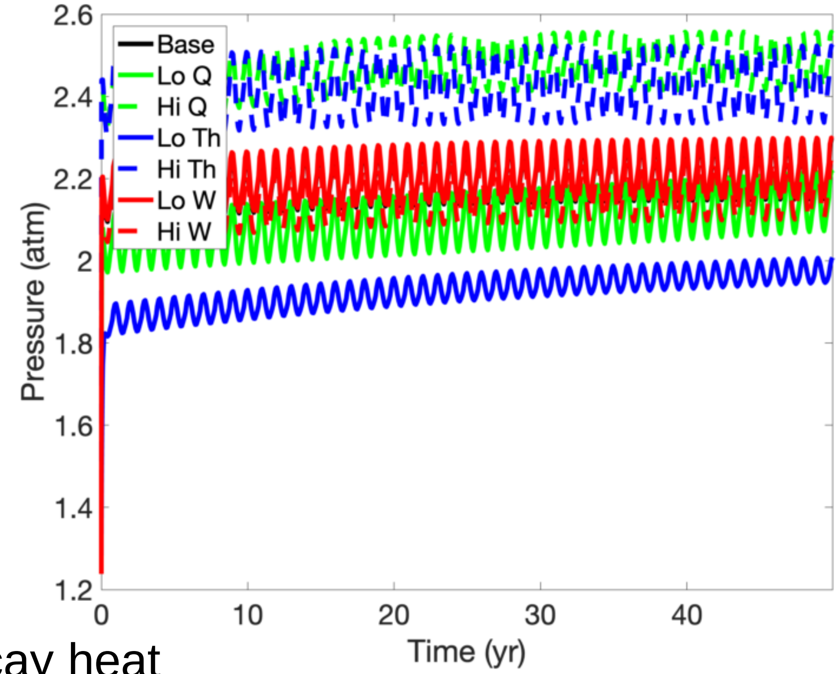


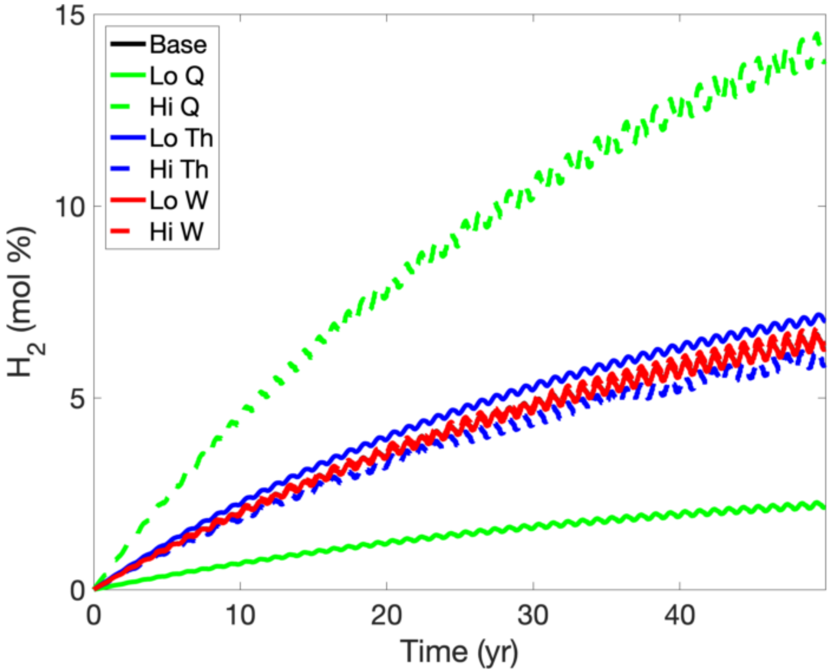


Order of magnitude
lower than canister limit

ATR Residual Pseudo-Boehmite Case

- Pressure variation higher, up to 2.5 atm max
- Hydrogen concentrations mostly unchanged, but slightly lower due to higher water vapor %
- Some dependence on oxide thickness due to water content
- High water content creates yearly fluctuations with more temperature dependence

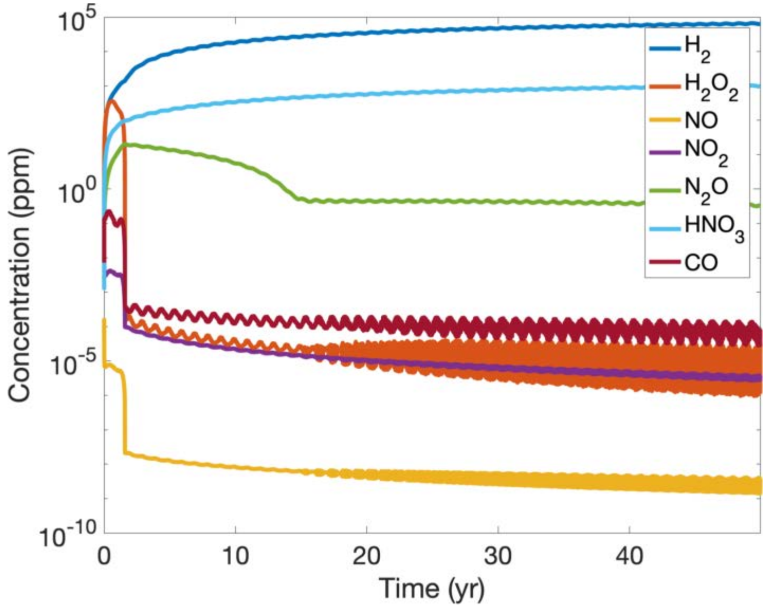


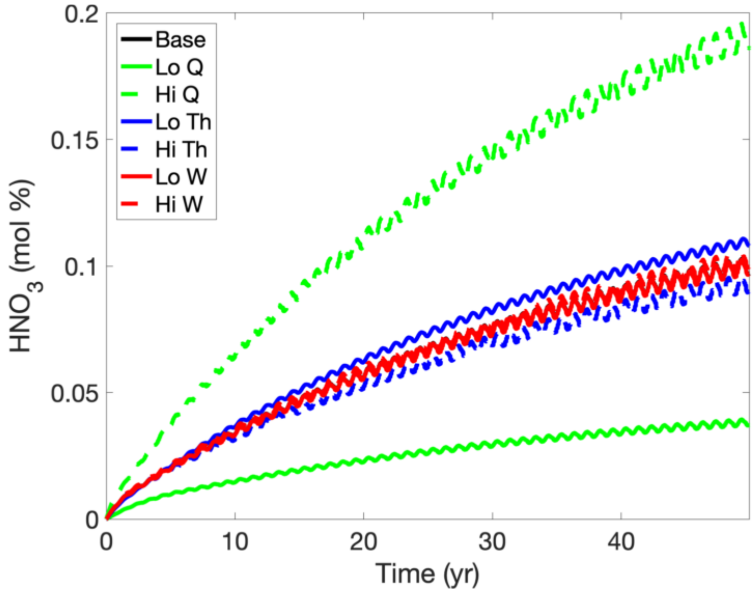


Q: Decay heat
Th: Oxide Thickness
W: Water content

ATR Residual Pseudo-Boehmite Case + 1% air

- Case with 1% residual air shows no significant changes in H_2 and total pressure from pure He case
- As with previous case, primarily HNO_3 as main additional component, nominal HNO_3 of 1000 ppm
  - Max of HNO_3 2000 ppm with high decay heat

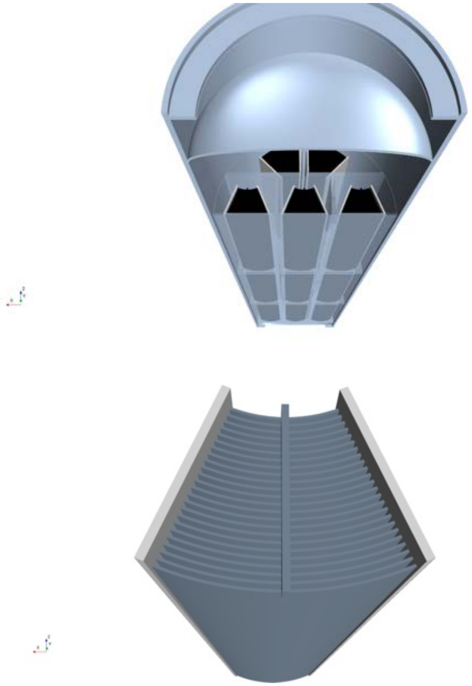


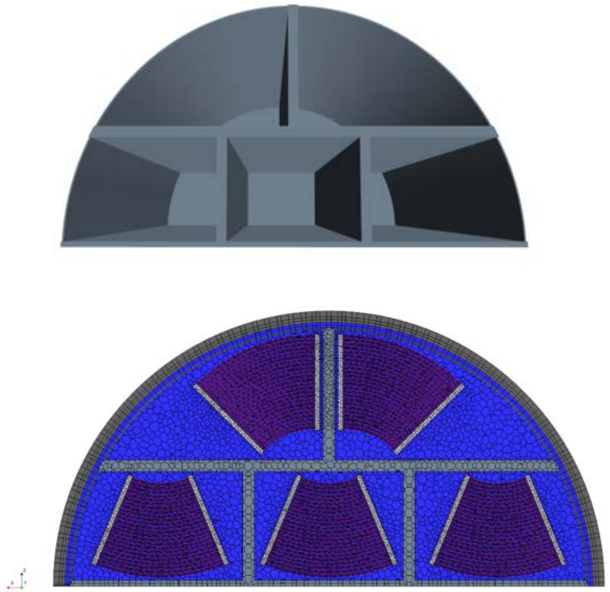


Q: Decay heat
Th: Oxide Thickness
W: Water content

Other ASNF

- MURR Fuel is also a significant quantity of DOE manage fuel
- Expected to be packed in Type-1a baskets in 10-foot-tall canisters
- Similar surface area to volume ratio as packaged ATR
  - Sensitivity to decay heat: 25/13.4/5 W (based on SRNL report[1])



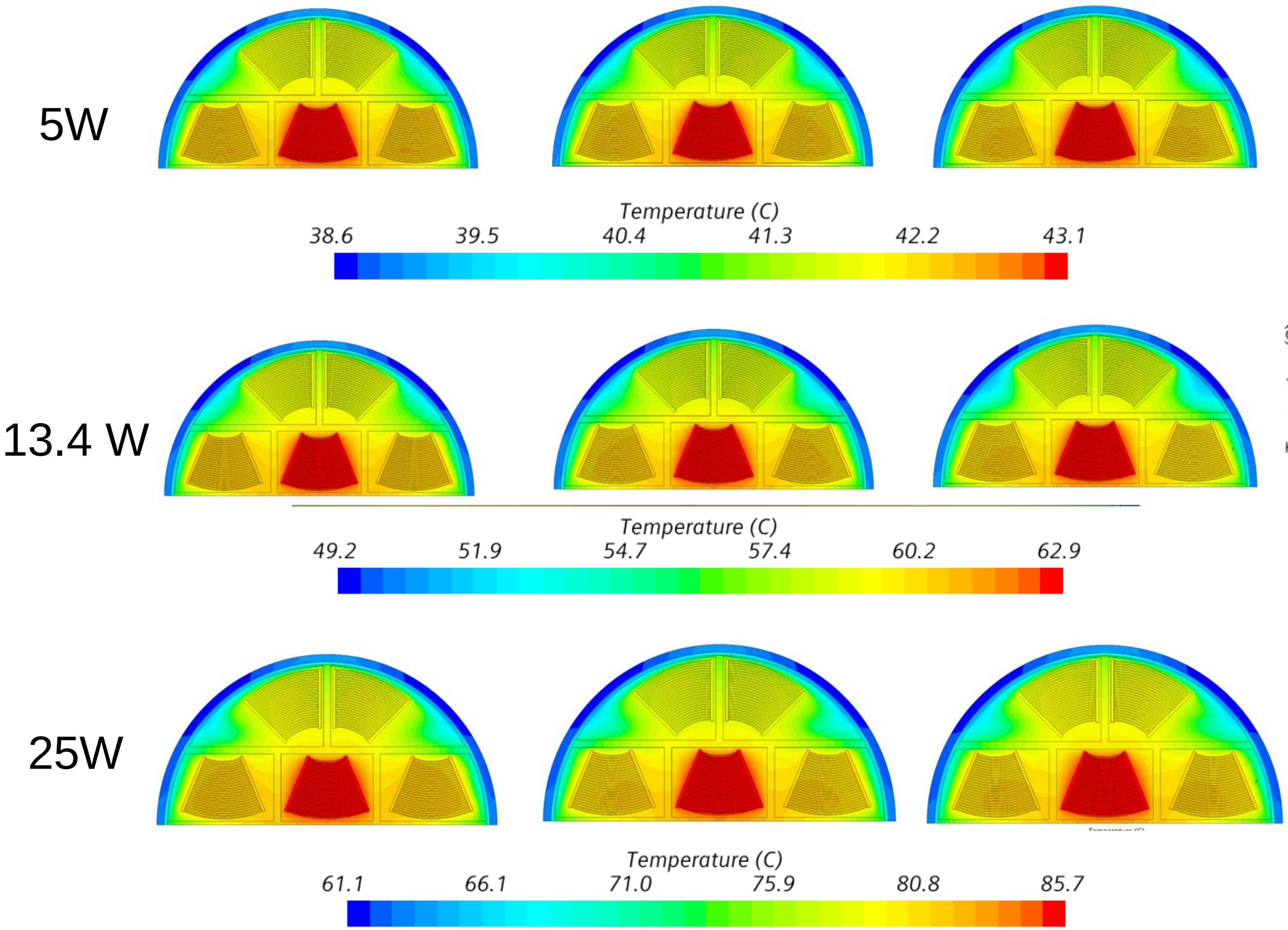


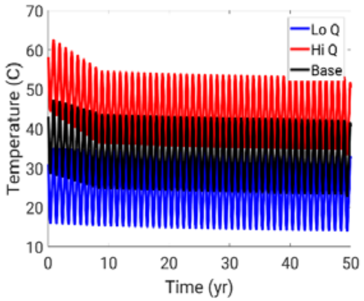
Configuration	Total Surf Area	Free Volume	Ratio
ATR 15 foot 18” D	120 m^2	450 L	0.267
MURR 10 foot 18” D	78.8 m^2	284 L	0.277

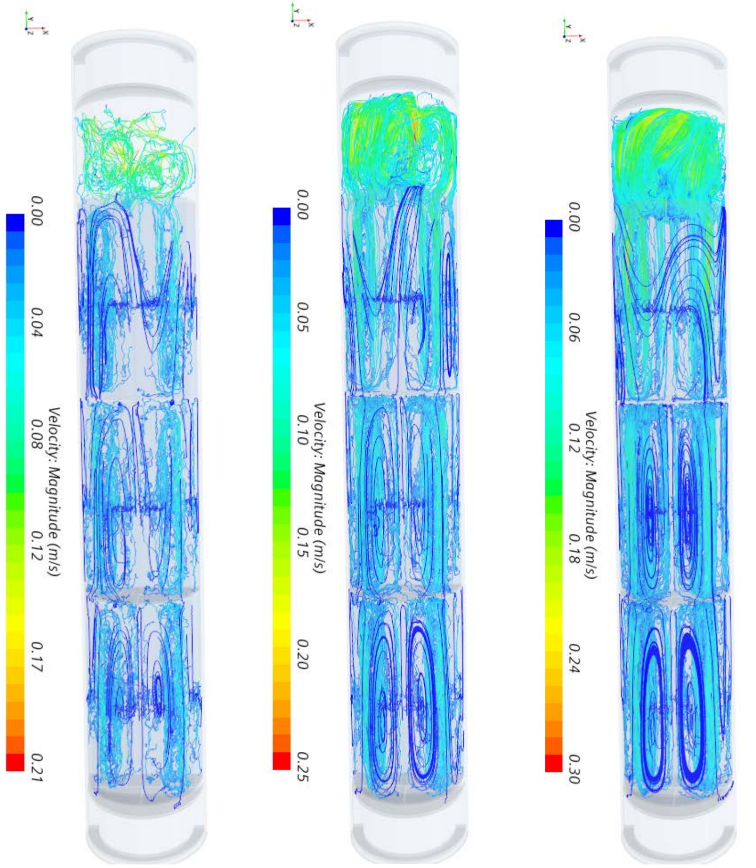
[1]Sindelar, R.L., Leeper, P.A., Dunsmil, M.D., 2012, “Reference Fuel Assembly for Dry Storage Demonstration of L-Basin Spent Fuel”, Tech. Rep. Savannah River National Laboratory, SRNL-TR-2012-00098.

MURR Fuel - Thermal

- Similar profiles to the ATR hottest in center



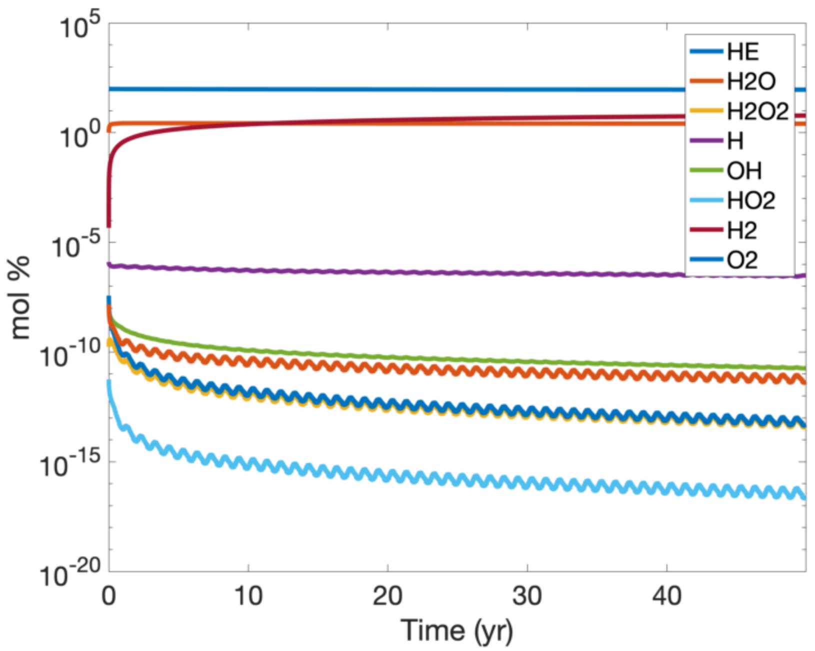


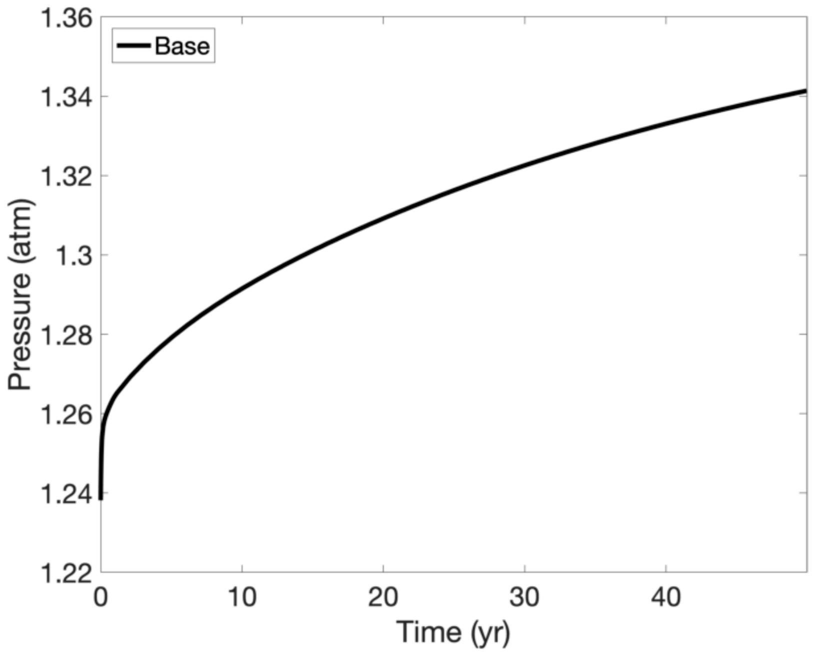


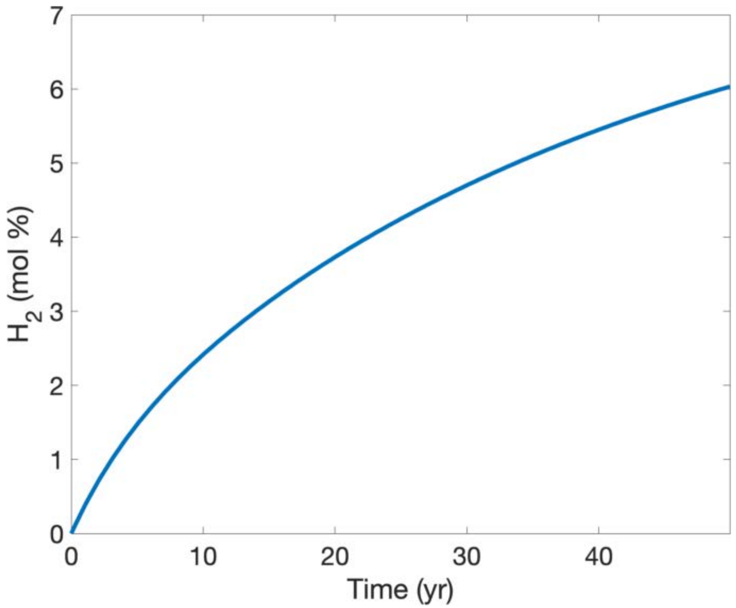
Increasing heat more recirculation

MURR Fuel - Chemistry

- Pressure and hydrogen in the MURR DOE sealed canister lower than ATR fuel for base case
  - As with ATR storage, no appreciable O_2
  - 1.34 atm and 6% H_2 for nominal case

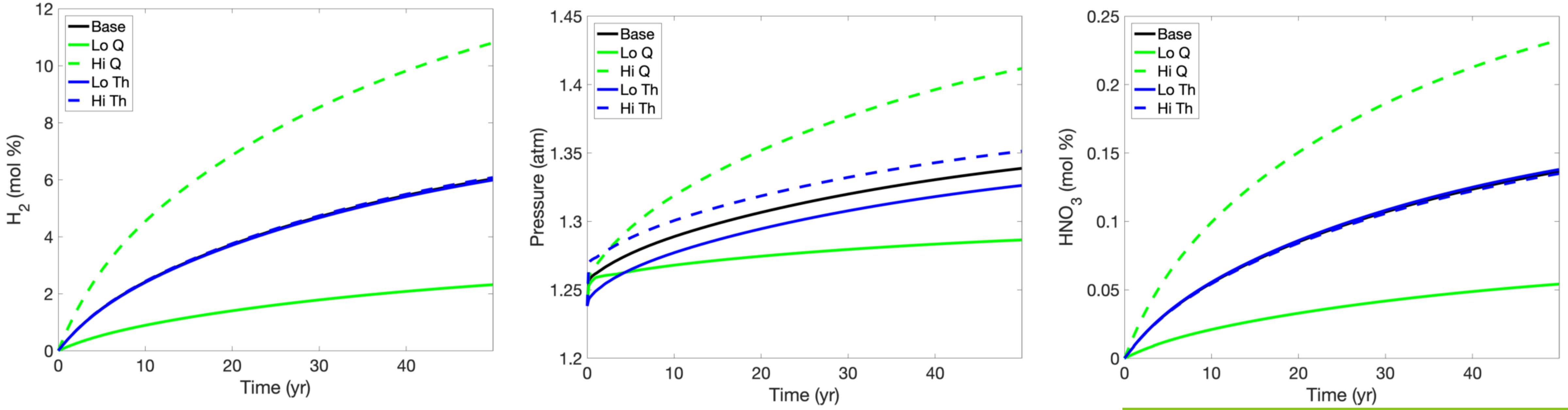






MURR Fuel - Chemistry

- Variation of decay heat shows values lower than ATR fuel
  - Max pressure: 1.41 atm
  - Max H_2: 10.8%
  - With residual Air: Max HNO_3 2300 ppm



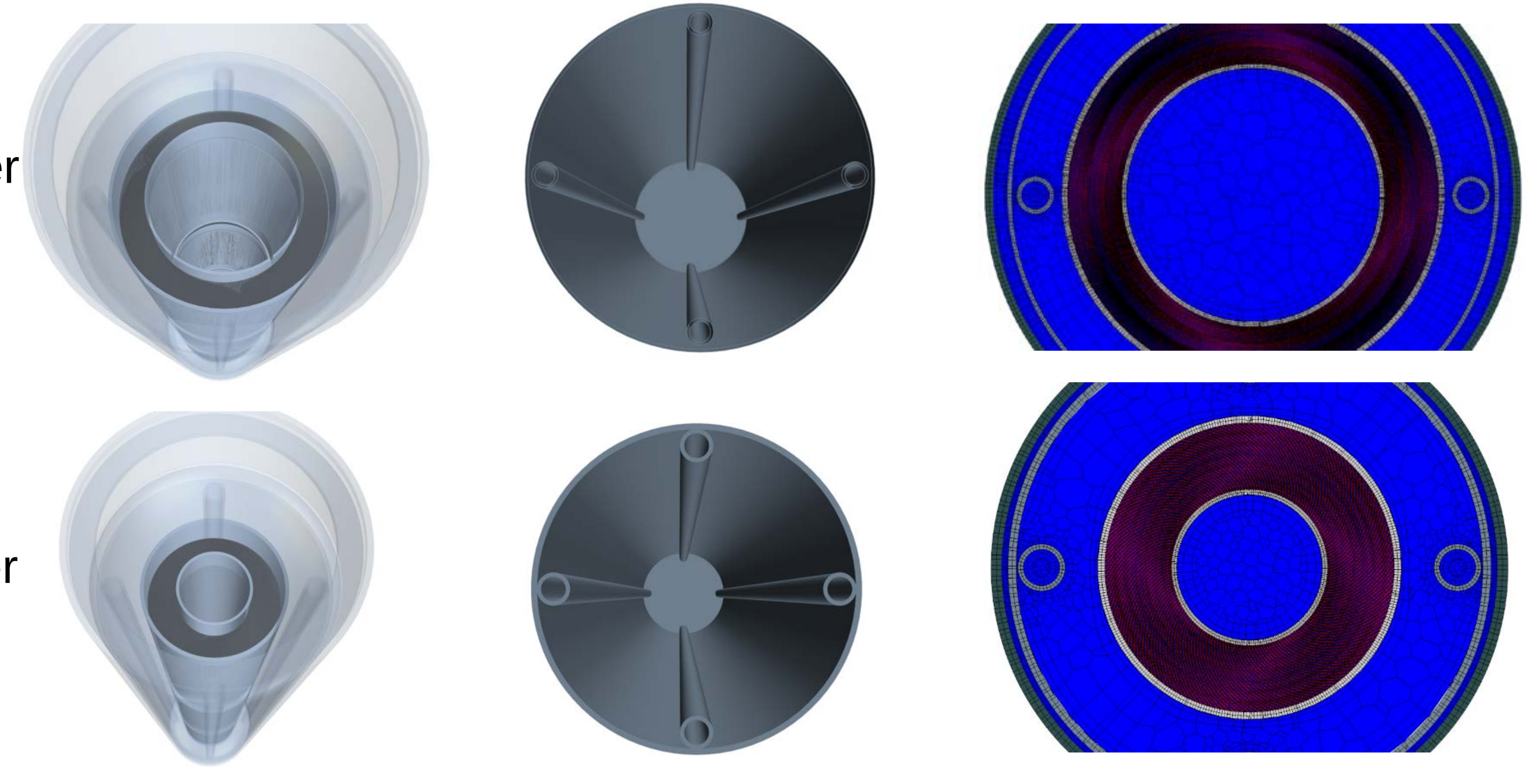
Q: Decay heat
Th: Oxide Thickness

HFIR Fuel

- The HFIR fuel specifications are expected to split the inner and outer annulus into two separate storage canisters with Type-6a/6b baskets
  - HFIR-Outer in 24” Diameter
  - HFIR-inner in 18” Diameter

HFIR-outer

HFIR-inner

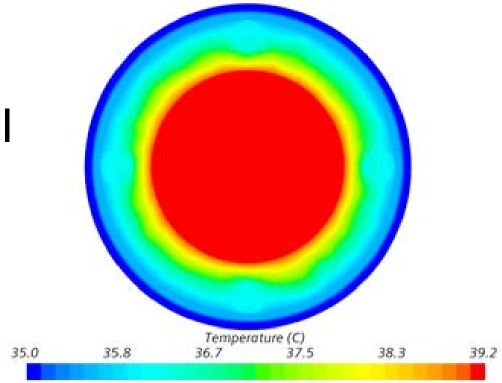


Configuration	Total Surface Area	Free Volume	Ratio
ATR 15 foot 18” D (reference)	120 m^2	450 L	0.267
HFIR-inner 10 foot 18” D	56.9 m^2	296 L	0.192
HFIR outer 10 foot 24” D	108.4 m^2	548 L	0.198

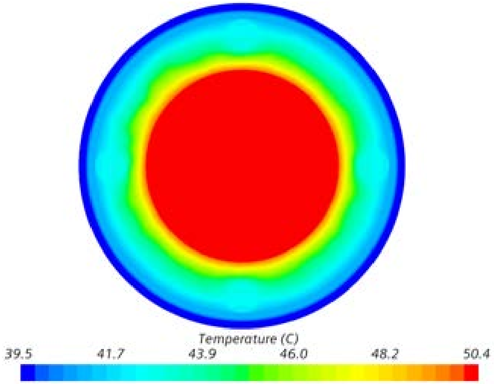
HFIR Fuel - Thermal

- Geometry of HFIR annulus results in central uniform central temperature
- Less horizontal packing density = 10-20 C colder than ATR layout

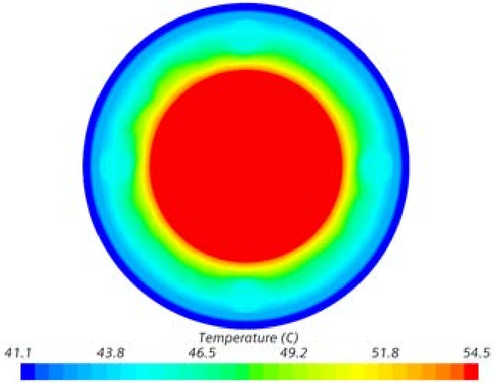
HFIR-I



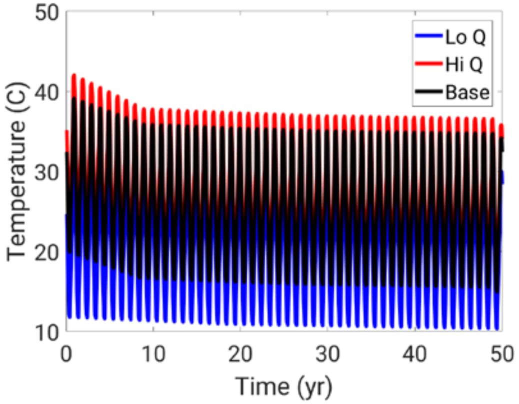
76 W



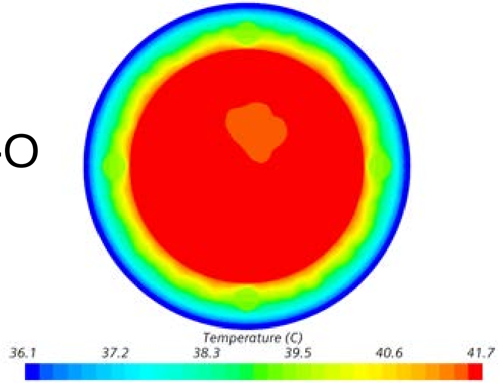
60 W



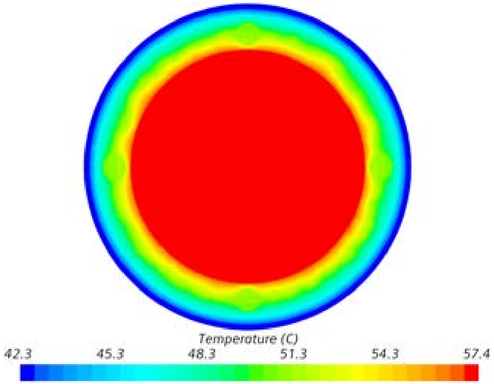
21 W



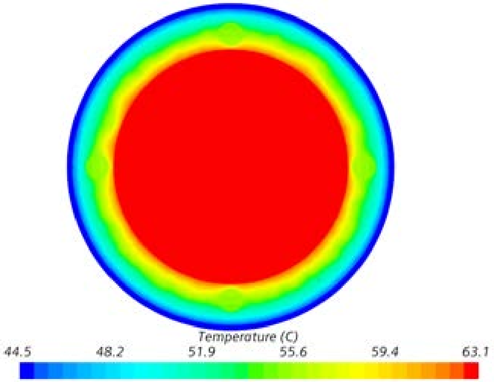
HFIR-O



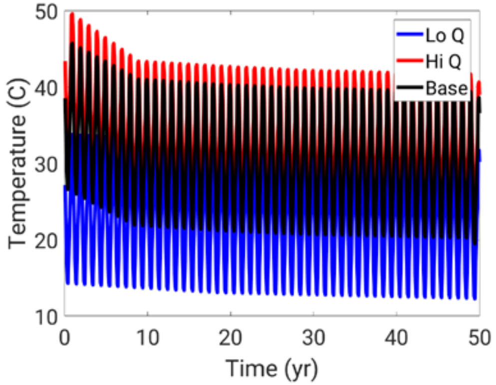
114 W



112 W

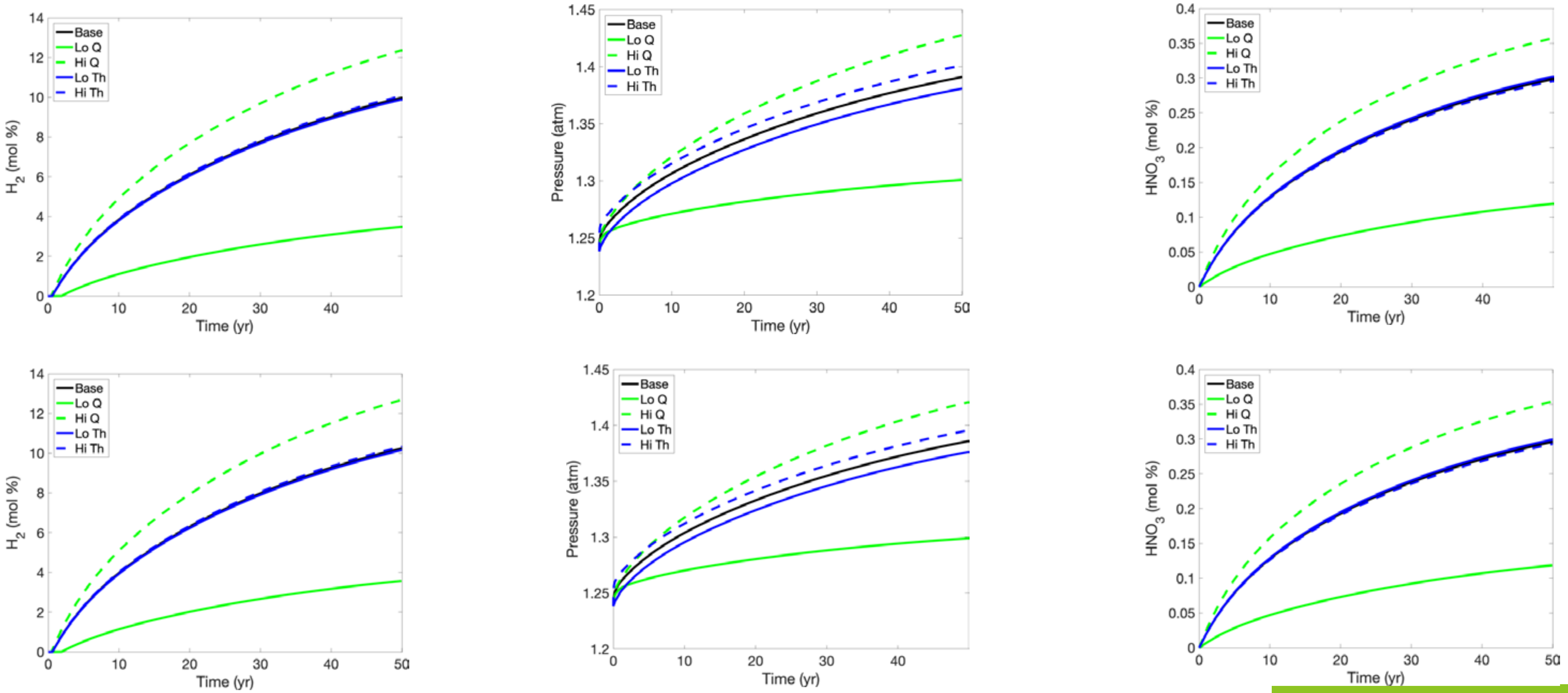


39 W



HFIR Fuel - Chemistry

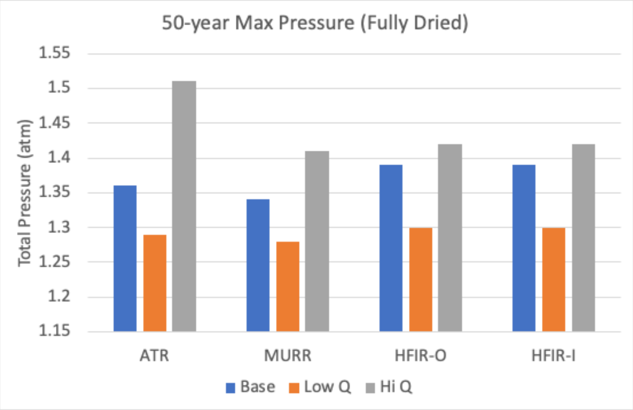
- Maximums for both inner/outer HFIR storage packages very similar
  - 12% mole H_2, 1.4 atm (dried), 2.17 atm (undried), 3500 HNO_3 (with residual air)
  - With larger surface area of HFIR, surface oxide thickness sensitivity remains small

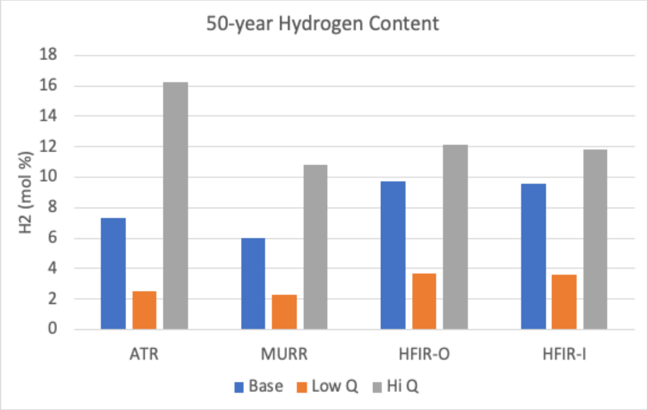


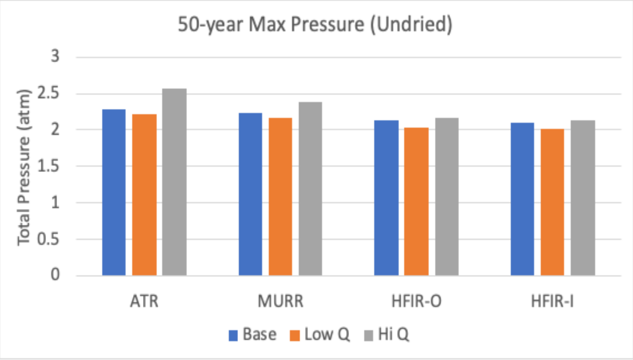
Q: Decay heat
Th: Oxide Thickness

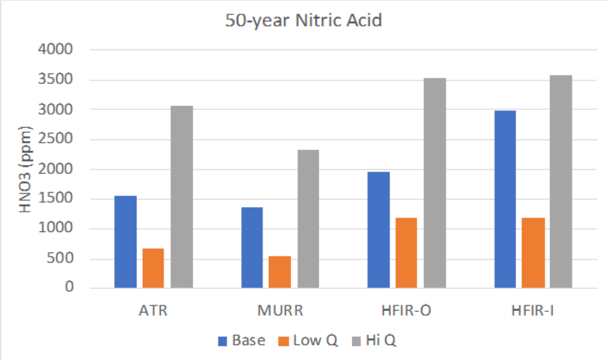
Packaging Scenario Summary

- ATR worst case bounds others
- Nominal cases of HFIR slightly higher P and H_2
  - Assumptions from tabulation of post-reactor removal vs. current inventory
- Lower temperatures + more air in HFIR allow for more nitric acid formation









Conclusions

- Most scenarios exhibit significant H_2 above lower flammability limit, no case shows this in combination any appreciable amount of O_2
  - Low decay-heat cases show H_2 lower than flammability limit (<4%)
  - ATR (6W), MURR (5W), HFIR-I (21W), HFIR-O (39W)
- If 1% residual air is present, possible for 500-3000 ppm HNO_3
  - Likely minimal corrosion (0.01-0.034 mpy) based on lit. survey
- Worst-case ATR fuel bounds MURR/HFIR models for H_2 and pressure
  - Maximum canister pressure 34 atm (500 psi)
  - Nominal scenario: 1.36 atm total pressure, 7% mole frac H_2
  - High decay heat: 1.51 atm total pressure, 16% mole frac H_2
  - High decay heat + undried: 2.6 atm total pressure, 15% mole frac H_2
- Changes with oxide thickness small across fuels modeled
  - Characterization on individual fuel basis likely unneeded

Future Goals

- In 1-year timeframe
- Update results if Al6061 alloy shows significant changes from Al1100
- Extended modeling timeframe beyond 50 years
- Adjust model as needed based on long-term radiolysis testing
  - Dried oxide samples show lower G-values than those used here
  - H_2 from SRNL “large plate” tests show a leveling off in production

- Validation with instrumented lid test on longer timeframe

Published reports

- INL/EXT-18-51683 Transient Coupled Chemical-Thermal-Fluid Field Simulation for Sealed Aluminum-clad Spent Nuclear Fuel Storage Canister
- INL/EXT-18-51681 Development of Transient Coupled Chemical-Thermal-Fluid Multiphysics Simulation for Unsealed, Vented Aluminum-clad Spent Nuclear Fuel Storage Canister
- INL/EXT-19-52650 Sensitivity Study of Coupled Chemical-CFD Simulations for Sealed and Unsealed Aluminum-clad Spent Nuclear Fuel Storage Canisters
- INL/EXT-19-55185 Full-scale Model of Dry Storage of Aluminum Clad Spent Nuclear Fuel
- INL EXT-20-57893 Modeling of SRS Aluminum-clad Spent Nuclear Fuel in Standard DOE Sealed Canisters
- INL EXT-20-59994 Chemical Modeling of ATR Fuel in DOE Standard Canisters with Borated Stainless Steel Corrosion
- INL EXT-21-62306 Modeling of ATR fuel in DOE Standard Canisters with Helium Backfilled Condition
- Sensitivity Study of Coupled Chemical-CFD Simulations for Analyzing Aluminum-clad Spent Nuclear Fuel Storage in Sealed Canisters submitted to *Nuclear Engineering and Design*

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Questions?

Physical parameters

Material	Density [kg/m3]	Thermal Conductivity [W/m K]	Heat Capacity [J/kg K]	Emissivity [-]
Al-6061 (siding/back plates)[i]	2702	167	896	0.82
Stainless Steel 304 (buckets)[ii]	7900	14.9	477	0.7
Stainless Steel 316 (canister)[ii]	8238	13.4	468	0.7
Carbon Steel (impact plates)[ii]	7854	60.5	434	0.89
ATR Fuel Plates[iii]	3680	42.6	614.0	0.82 (assumed)

[i]. S.T. Polkinghorne and J.M. Lacy, “Thermophysical and Mechanical Properties of ATR Core Materials,” Report No. PG-T-91-031, EG&G Idaho Inc (1991).
[ii]. F.P. Incropera, D.P. DeWitt, T.L. Bergman, and A.S. Lavine, *Fundamentals of Heat and Mass Transfer*, *Sixth Edition*, John Wiley and Sons, Hoboken, NJ (2007).
[iii]. D.B. Illum, “ATR Fuel Summary Report,” Tech. Report INEL-96/300 (1996).

Dried ATR Fuel

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 10um thickness, 1% H2O(g))	1.36	7.3	3e-8	1.36	7.4	0.21	1562
Low decay heat (6W)	1.29	2.5	1,6e-8	1.29	2.2	0.21	565
High decay heat (42W)	1.51	16.2	7e-8	1.50	16.7	0.21	3070
Low Thickness (5 µm)	1.35	7.3	3e-8	1.34	7.3	0.21	1581
High Thickness (15 µm)	1.37	7.4	3e-8	1.37	7.4	0.21	1545

Residual Pseudo-Boehmite Case

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 1% H2O(g))	2.29	6.7	2e-7	2.29	6.7	0.21	1028
Low decay heat (6W)	2.21	2.3	1e-7	2.21	2.1	0.21	394
High decay heat (42W)	2.56	14.5	6e-7	2.56	14.8	0.21	1957
Low H2O% (.1%)	2.29	6.6	2e-7	2.30	6.7	0.21	1025
High H2O% (10%)	2.25	6.8	2e-7	2.25	6.9	0.21	1057
Low Thickness (5 µm)	2.0	7.2	5e-8	2.0	7.2	0.21	1108
High Thickness (15 µm)	2.52	6.3	5e-7	2.52	6.3	0.21	963

Dried MURR Fuel

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 10um thickness, 1% H2O(g))	1.34	6.0	4e-8	1.34	6.0	0.21	1363
Low decay heat (6W)	1.29	2.3	2e-8	1.29	2.1	0.21	541
High decay heat (42W)	1.41	10.8	6e-8	1.41	11.0	0.21	2325
Low Thickness (5 µm)	1.33	6.0	4e-8	1.33	6.0	0.21	1379
High Thickness (15 µm)	1.35	6.1	4e-8	1.35	6.0	0.21	1349

Residual Pseudo-Boehmite Case

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 1% H2O(g))	2.24	5.5	2e-7	2.24	5.5	0.21	911
Low decay heat (6W)	2.16	2.2	1e-7	2.16	2.0	0.21	389
High decay heat (42W)	2.38	9.9	4e-7	2.38	10.0	0.21	1537
Low H2O% (.1%)	2.25	5.5	2e-7	2.25	5.5	0.21	908
High H2O% (10%)	2.20	5.6	2e-7	2.19	5.6	0.21	939
Low Thickness (5 µm)	1.96	5.9	5e-8	1.96	5.9	0.21	977
High Thickness (15 µm)	2.49	5.2	5e-7	2.48	5.2	0.21	858

Dried HFIR-Outer Fuel

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 10um thickness, 1% H2O(g))	1.39	9.9	6e-8	1.39	10.3	0.21	2961
Low decay heat (6W)	1.30	3.7	4e-8	1.03	3.6	0.21	1184
High decay heat (42W)	1.43	12.1	8e-8	1.43	12.7	0.21	3536
Low Thickness (5 µm)	1.38	9.8	7e-8	1.38	10.2	0.21	2993
High Thickness (15 µm)	1.40	10.0	6e-8	1.40	10.3	0.21	2932

Residual Pseudo-Boehmite Case

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 1% H2O(g))	2.13	9.6	3e-7	2.14	9.9	0.21	2081
Low decay heat (6W)	2.03	3.5	2e-7	2.03	3.5	0.21	856
High decay heat (42W)	2.17	11.9	3e-7	2.17	12.2	0.21	2490
Low H2O% (.1%)	2.14	9.6	3e-7	2.14	9.8	0.21	2074
High H2O% (10%)	2.09	9.8	3e-7	2.42	10.5	0.21	3798
Low Thickness (5 µm)	1.87	10.3	8e-8	1.87	10.6	0.21	2228
High Thickness (15 µm)	2.32	9.1	7e-7	2.32	9.3	0.21	1970

Dried HFIR-inner Fuel

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 10um thickness, 1% H2O(g))	1.39	9.6	6e-8	1.38	10.0	0.21	2989
Low decay heat (6W)	1.30	3.6	4e-8	1.29	3.5	0.21	1194
High decay heat (42W)	1.42	11.8	7e-8	1.42	12.4	0.21	3576
Low Thickness (5 µm)	1.37	9.5	6e-8	1.37	9.9	0.21	3019
High Thickness (15 µm)	1.39	9.7	6e-8	1.39	10.0	0.21	2960

Residual Pseudo-Boehmite Case

	Sealed			Sealed + 1% air			
Case / Variable Max	Pressure (atm)	H_2 (%)	O_2 (%)	Pressure (atm)	H_2 (%)	O_2 (%)	HNO_3 (ppm)
Base (18W, 1% H2O(g))	2.10	9.4	2e-7	2.1	9.7	0.21	2119
Low decay heat (6W)	2.01	3.5	2e-7	2.01	3.4	0.21	869
High decay heat (42W)	2.14	11.7	2e-7	2.14	12.0	0.21	2539
Low H2O% (.1%)	2.11	9.4	2e-7	2.11	9.7	0.21	2112
High H2O% (10%)	2.05	9.7	3e-7	2.16	13.7	0.21	3494
Low Thickness (5 µm)	1.85	10.1	7e-8	1.85	10.4	0.21	2266
High Thickness (15 µm)	2.28	8.9	5e-7	2.28	9.2	0.21	2009