GAS-COOLED REACTOR
ADVANCED REACTOR TECHNOLOGIES PROGRAM

16 July 2024

AGR-3/4 PIE and Data Analysis

Adriaan Riet

AGR 3/4 Modeling and PIE

DOE ART GCR Review Meeting

Hybrid Meeting at INL

July 16–18, 2024

Cesium

- Transport model uses best-fit Henrian isotherm parameters
  - Quantities of fission products of interest are low enough to avoid the Freundlich isotherm's transition region, and are low enough (maximum of ppm concentration) that multi-layer adsorption is improbable
- Material properties considered
  - $D = D_0 \exp\left(-\frac{E_a}{RT}\right)$
  - $k_{sorption} = f_0 \exp\left(-\frac{k_H}{RT}\right)$
- Absolute vapor pressure has no impact on the dynamics of transport, so f_0 is used as a scaling factor to minimize numerical error

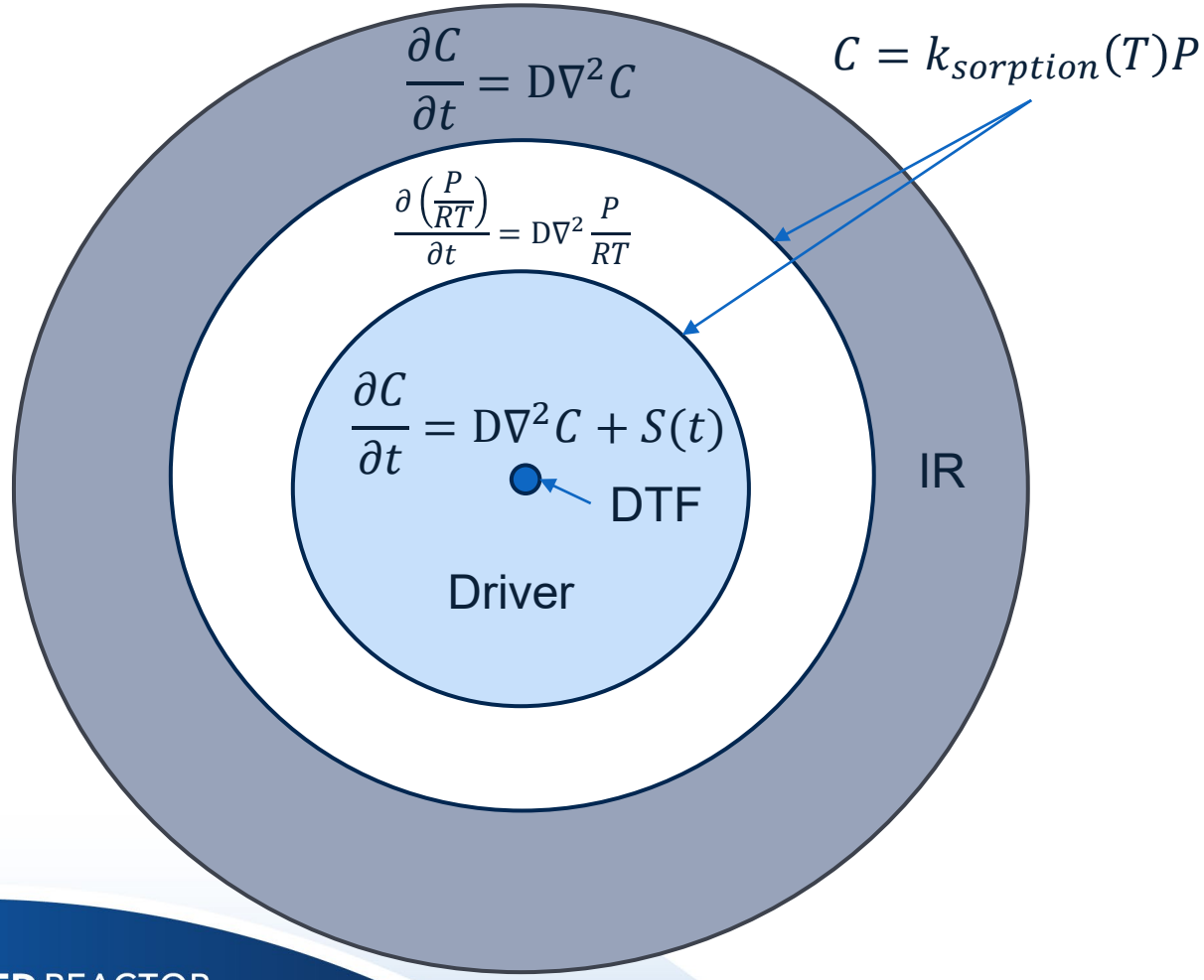
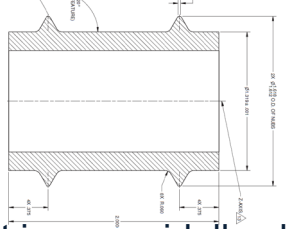
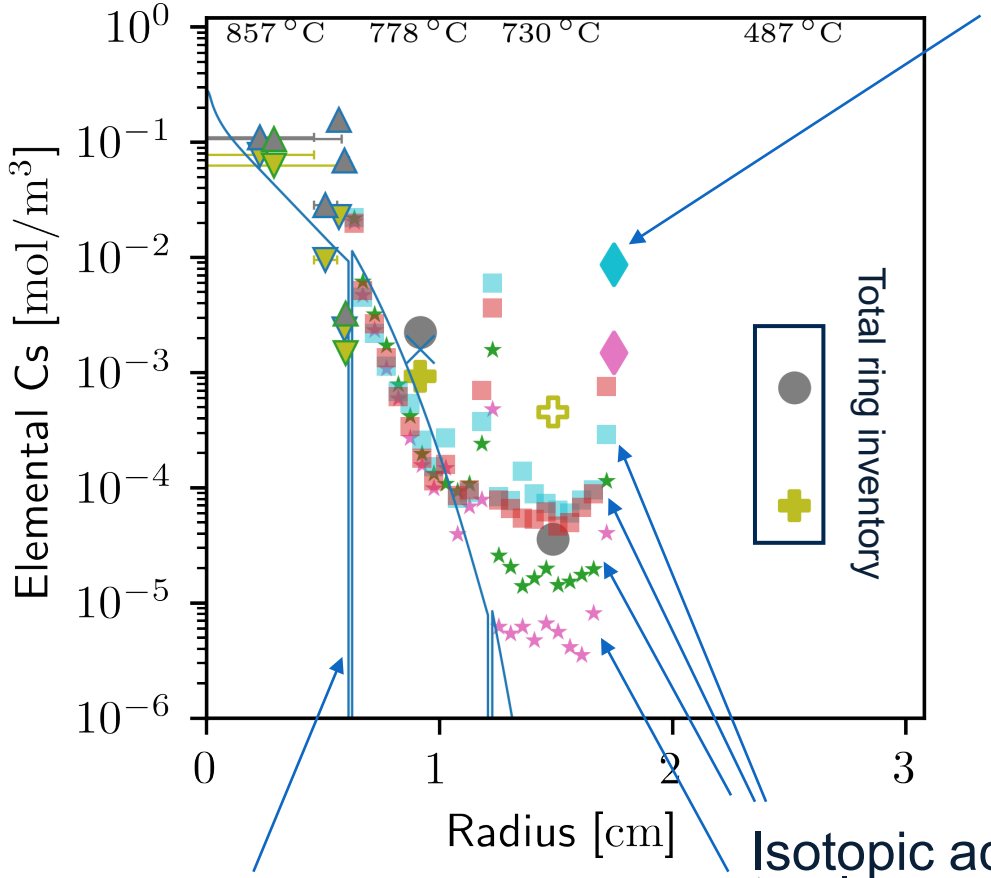
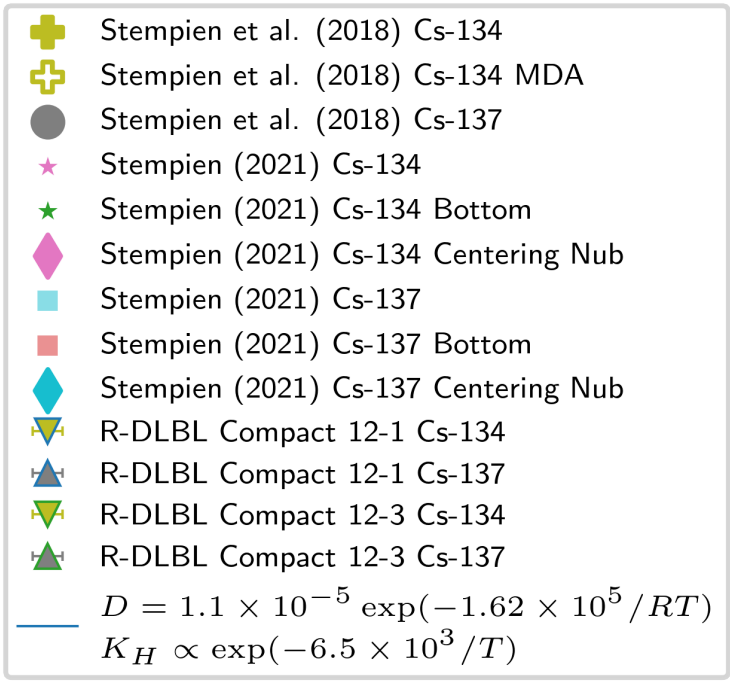


Figure description (Capsule 12)



Concentration of fission product in pyramidally-shaped protrusions used for centering the outer ring (outside surface of outer ring, with a higher surface-area to volume ratio)

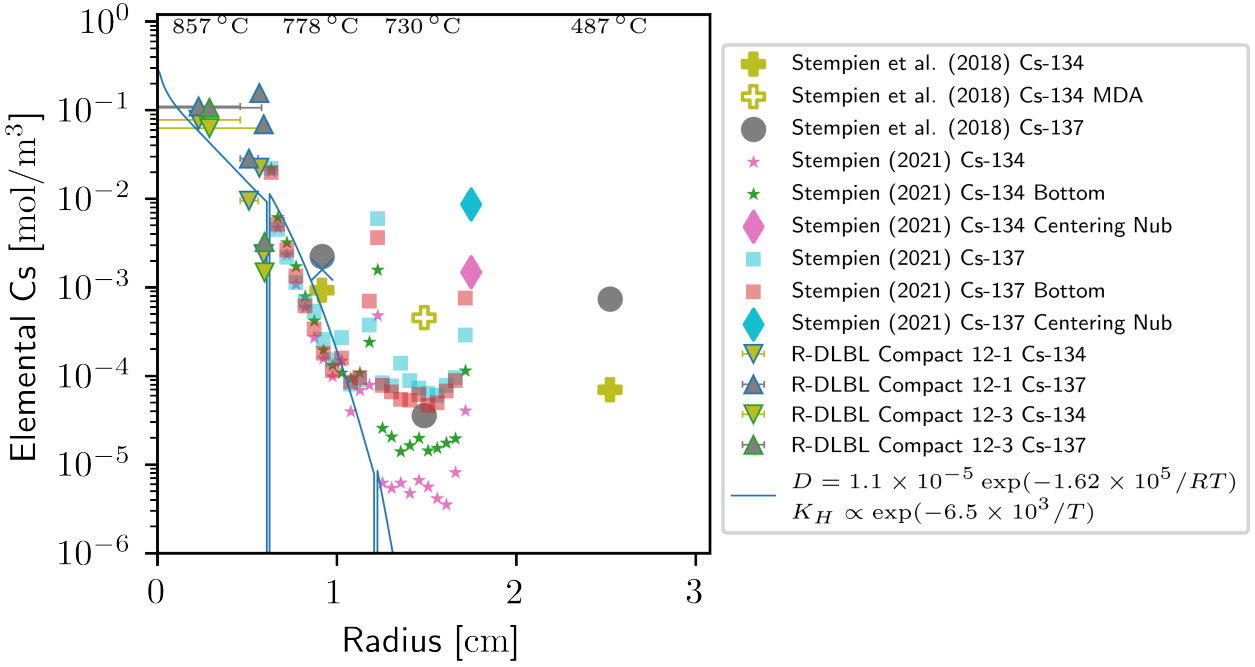




Best-fit numerical model, showing compact and ring boundaries

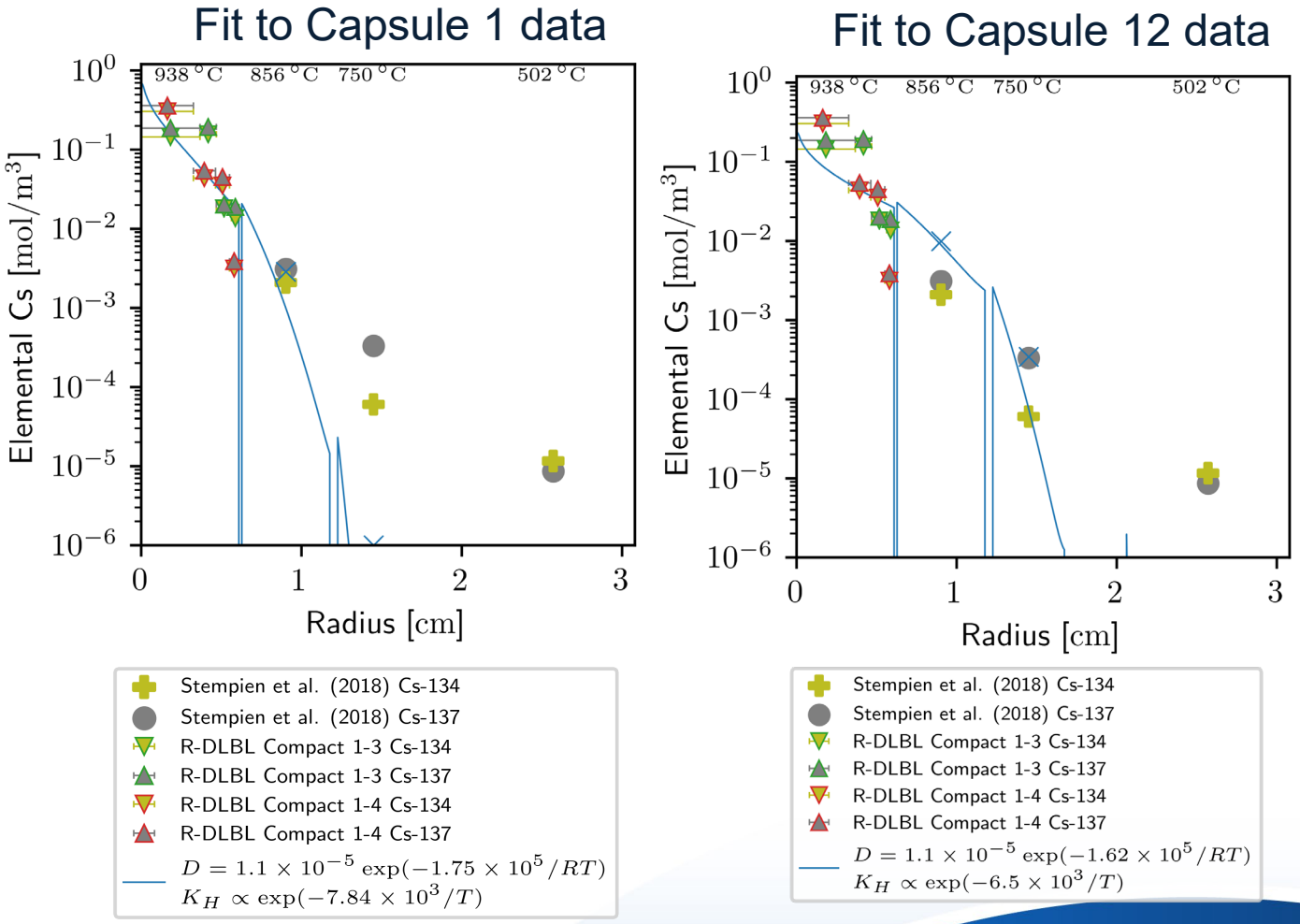
Isotopic activity profile from destructive analysis converted to elemental concentration in mol/m^3 (see legend for location)

Capsule 12



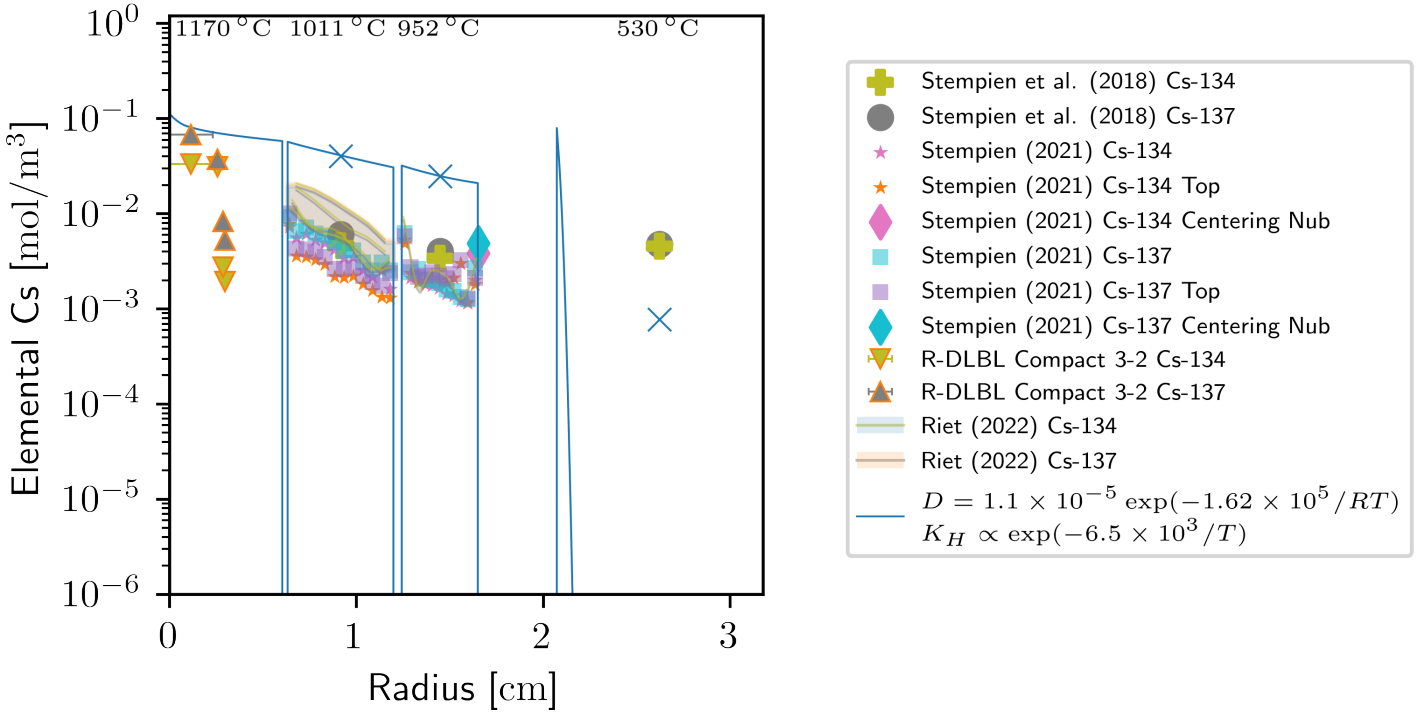
- Capsule 12 was one of the cooler capsules with a large amount of concentration data
- Outer ring concentration profile was not used for data fitting
  - Outer ring profile does not follow the functional form of pure temperature dependent diffusion – this would complicate fitting analysis
  - This may lead to underestimation of transport for low temperature regimes
- Capsule 12 cesium transport fit parameters seem to compare favorably when applied to other capsules
- Best estimate diffusivity and sorption
  - $D_0 = 1.1 \times 10^{-5} m^2/s$
  - $E_a \approx 162\ kJ/mol$
  - $K_H \approx 6.5\ kJ/mol$

Capsule 1



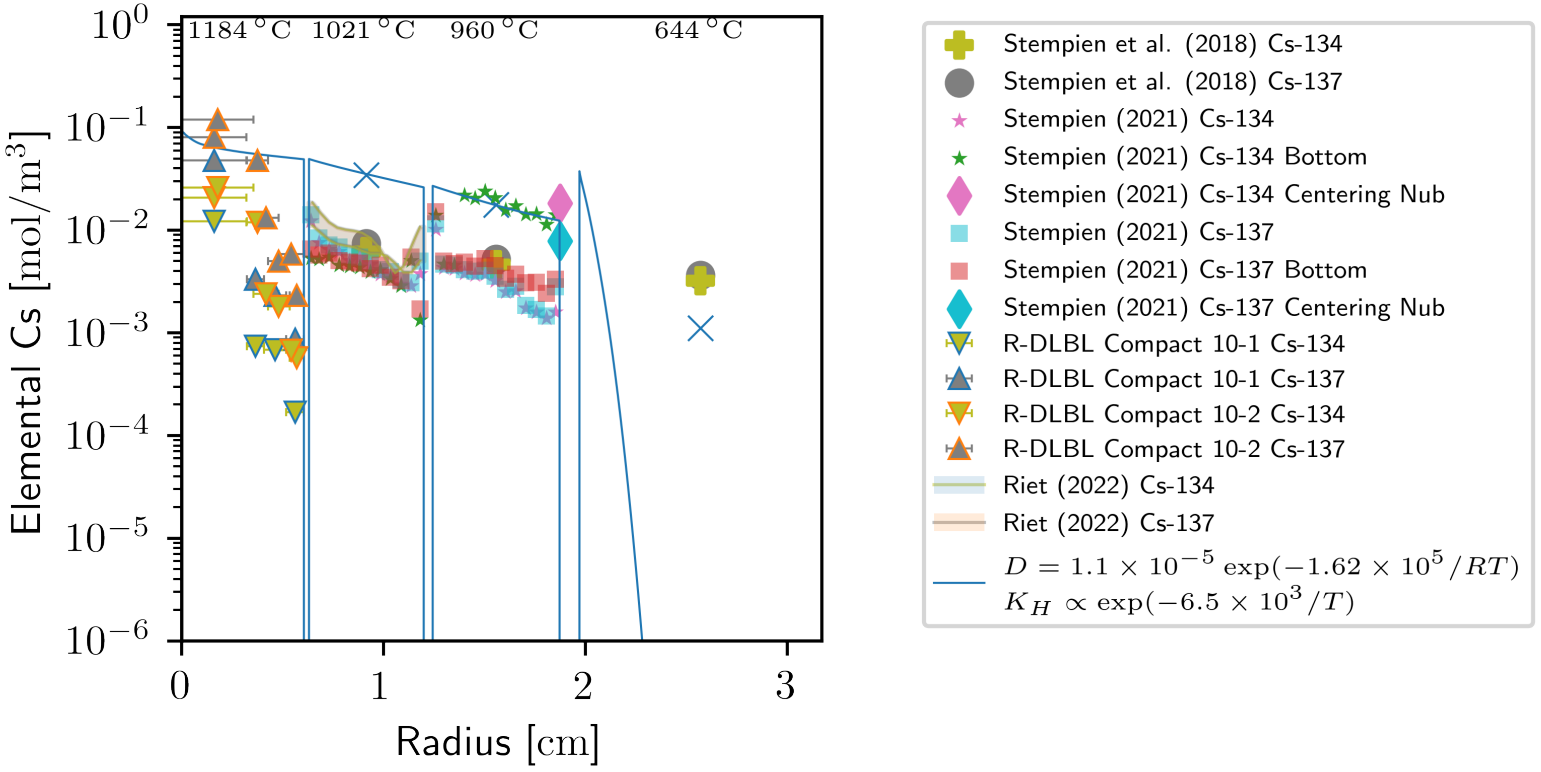
- Colder capsule
- Cs-134 considered reliable
- Best estimate diffusivity and sorption
  - $D_0 = 1.1 \times 10^{-5} m^2/s$
  - $E_a \approx 175\ kJ/mol$
  - $K_H \approx 7.8\ kJ/mol$
- Numerical fit to data from capsule 12 is more conservative, still underpredicts transport to the SR.

Capsule 3



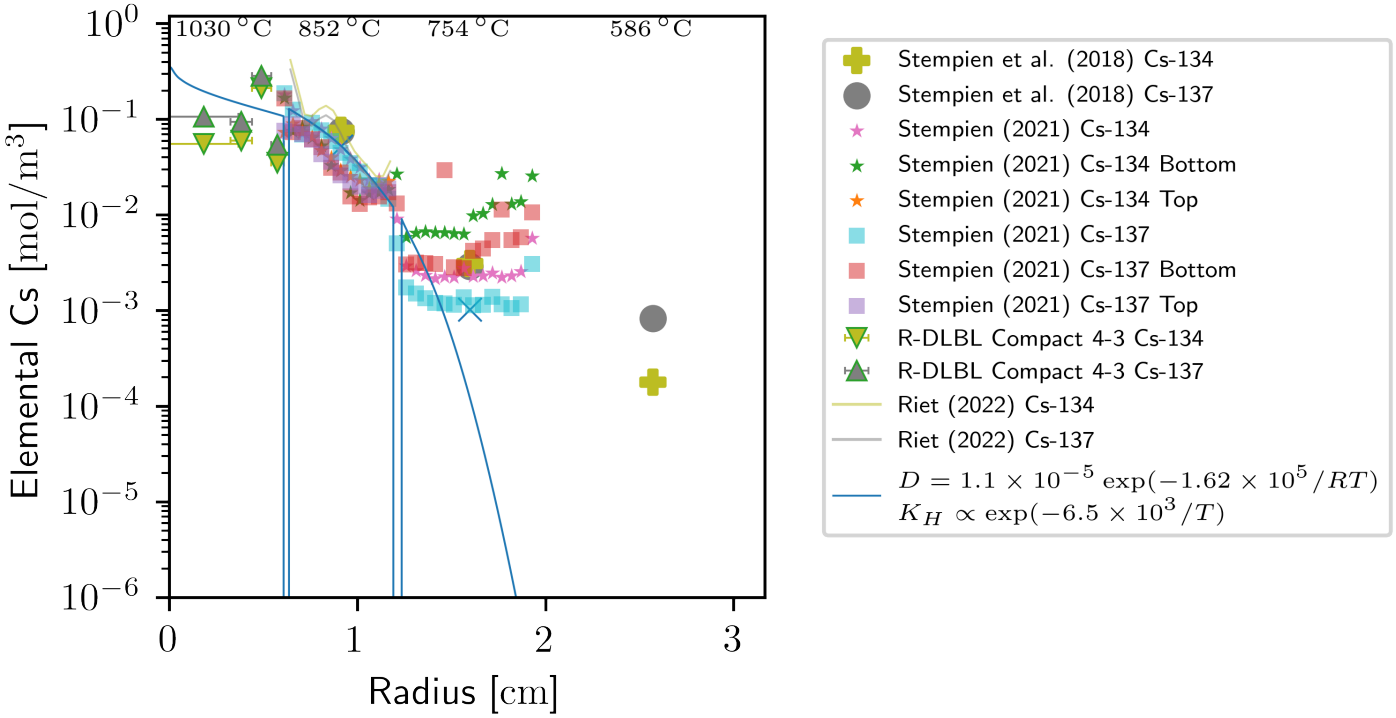
- One of the highest temperature capsules
- Transport model with capsule 12 fit parameters underpredicts transport to the sink ring (overpredicts within ring), but is still able to predict SR concentration to within an order of magnitude

Capsule 10



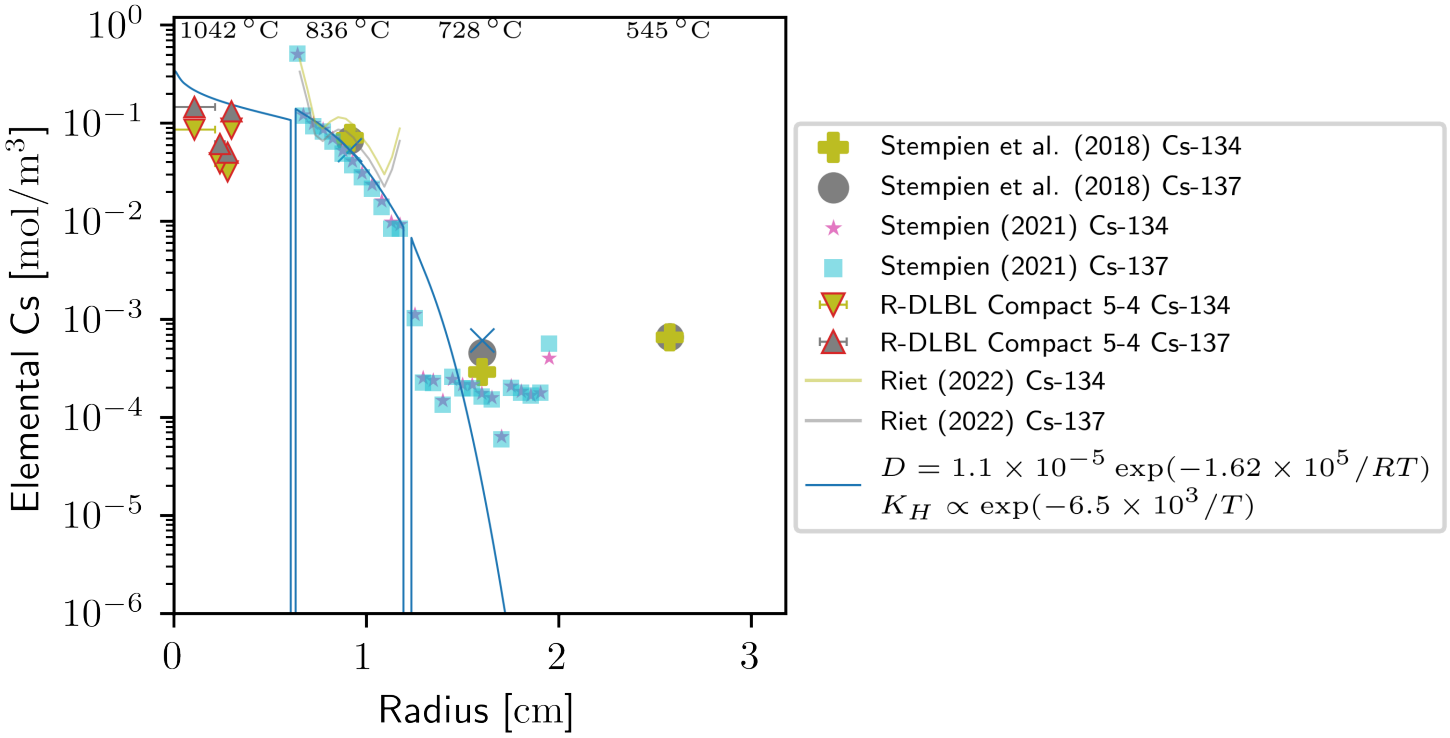
- Compact transport overpredicted
- IR transport seems slightly overpredicted
- OR transport seems accurate
- SR concentration predicted within a factor of 10
- PCEA IR

Capsule 4



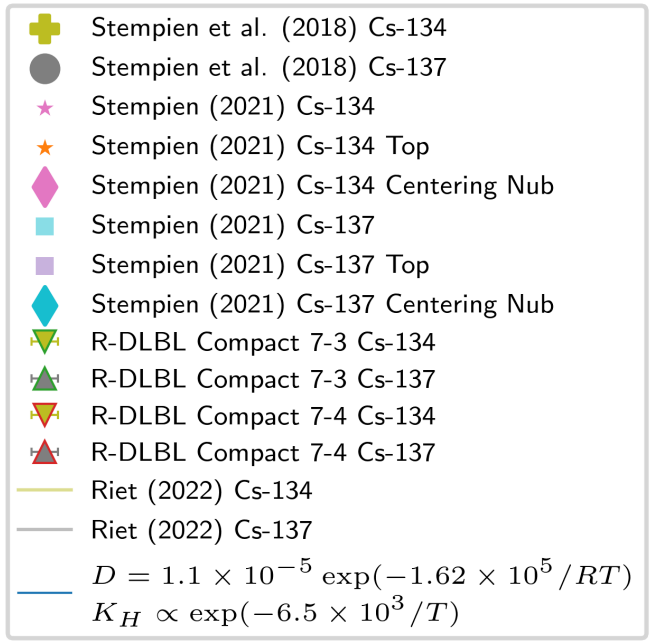
- Compact and SR temperature like capsule 3, but with IR/OR 200 °C cooler
- Compact transport seems to be predicted accurately
- IR transport matches quite well with experiment
- OR transport predicted to within a factor of 10
- SR inventory not predicted accurately

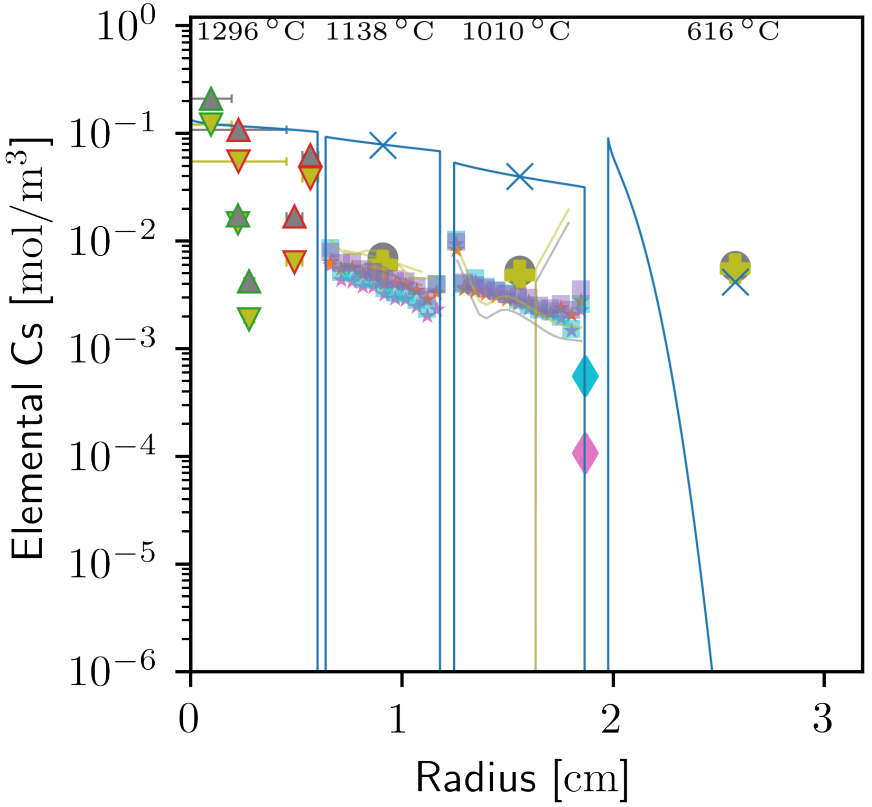
Capsule 5



- Transport model with Capsule 12 fit parameters does exceptionally well at predicting compact, IR and OR concentrations.
- Unable to predict SR concentrations, likely due to the faster low-temperature transport in the SR.

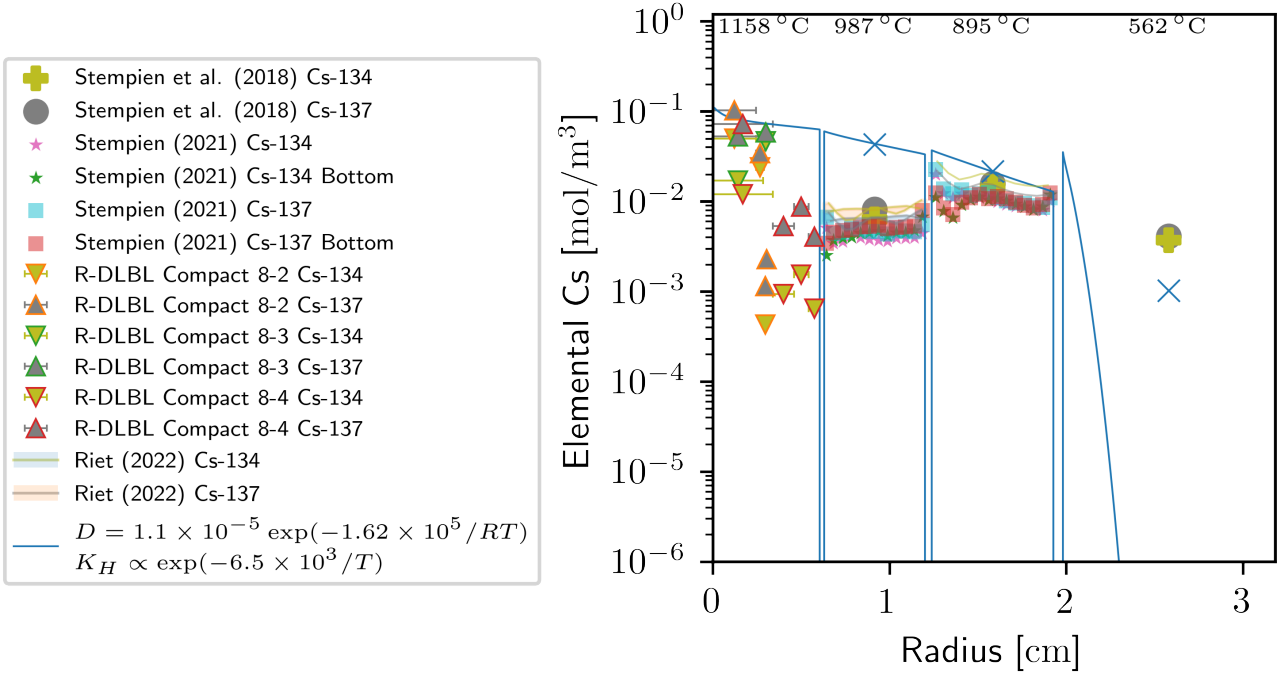
Capsule 7





- Transport model overpredicts transport within-rings, but predicts SR concentration accurately
- Nubs in this capsule do not show elevated concentrations of cesium, a deviation from other capsule behavior

Capsule 8

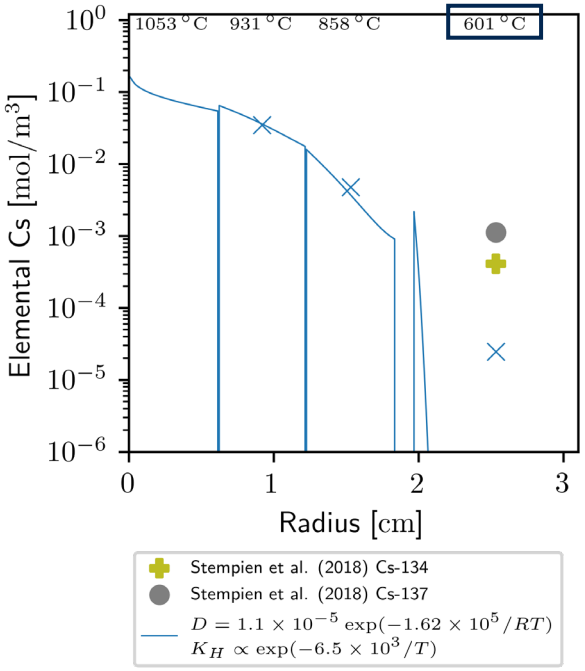


- Compact transport greatly overpredicted
- IR transport seems to be underpredicted
- OR transport seems to follow the same concentration profile, seems to be accurately predicted
- SR inventory predicted within a factor of ten
- IG-110 IR

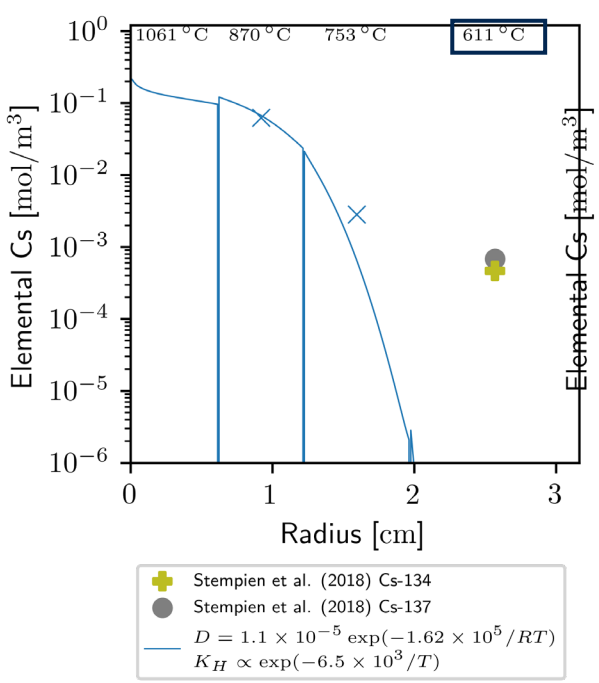
Capsules without Inner/Outer Ring data

Sink ring inventory is underpredicted by the model

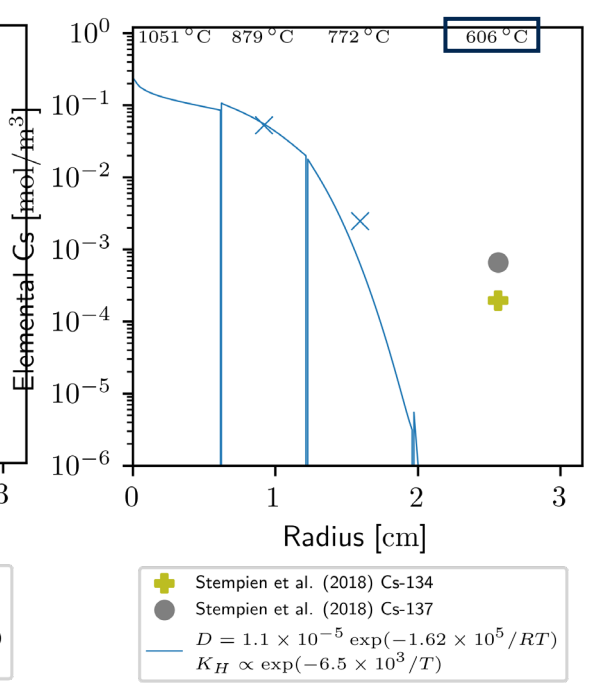
Capsule 2



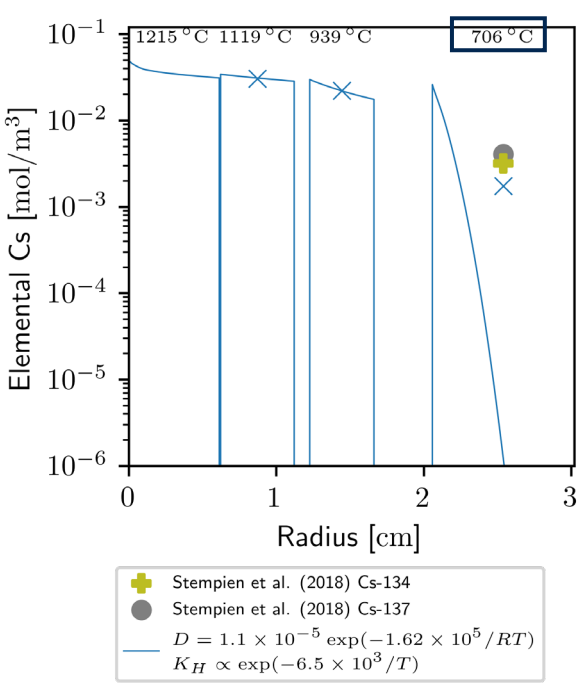
Capsule 6



Capsule 9

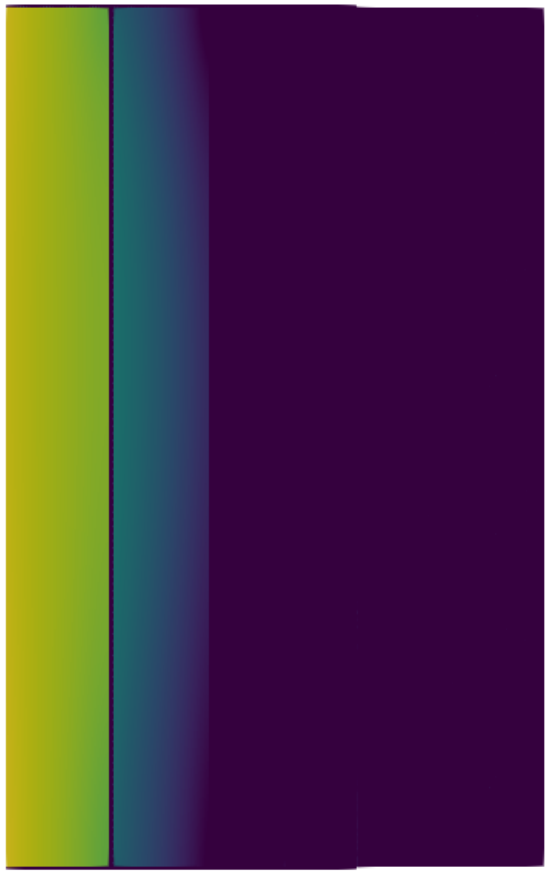


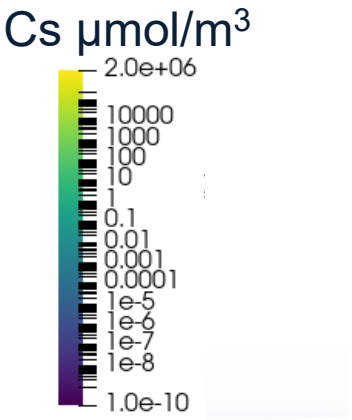
Capsule 11

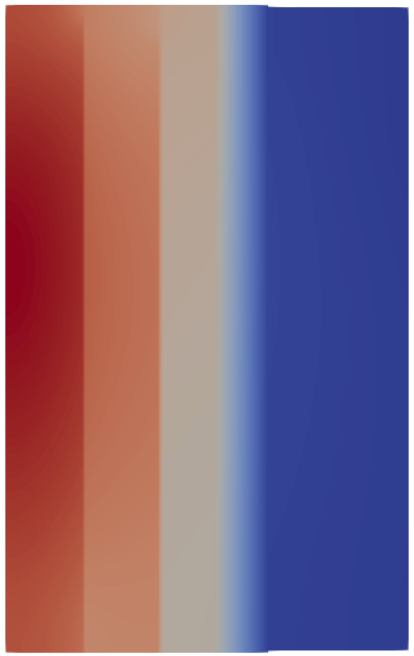


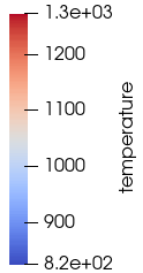
2D Modeling efforts

- Very preliminary
- 2D Diffusion only – 10^{-7} m^2/s
- Concentration profile does vary somewhat as a function of axial height
- 0.175mm gap on top and bottom





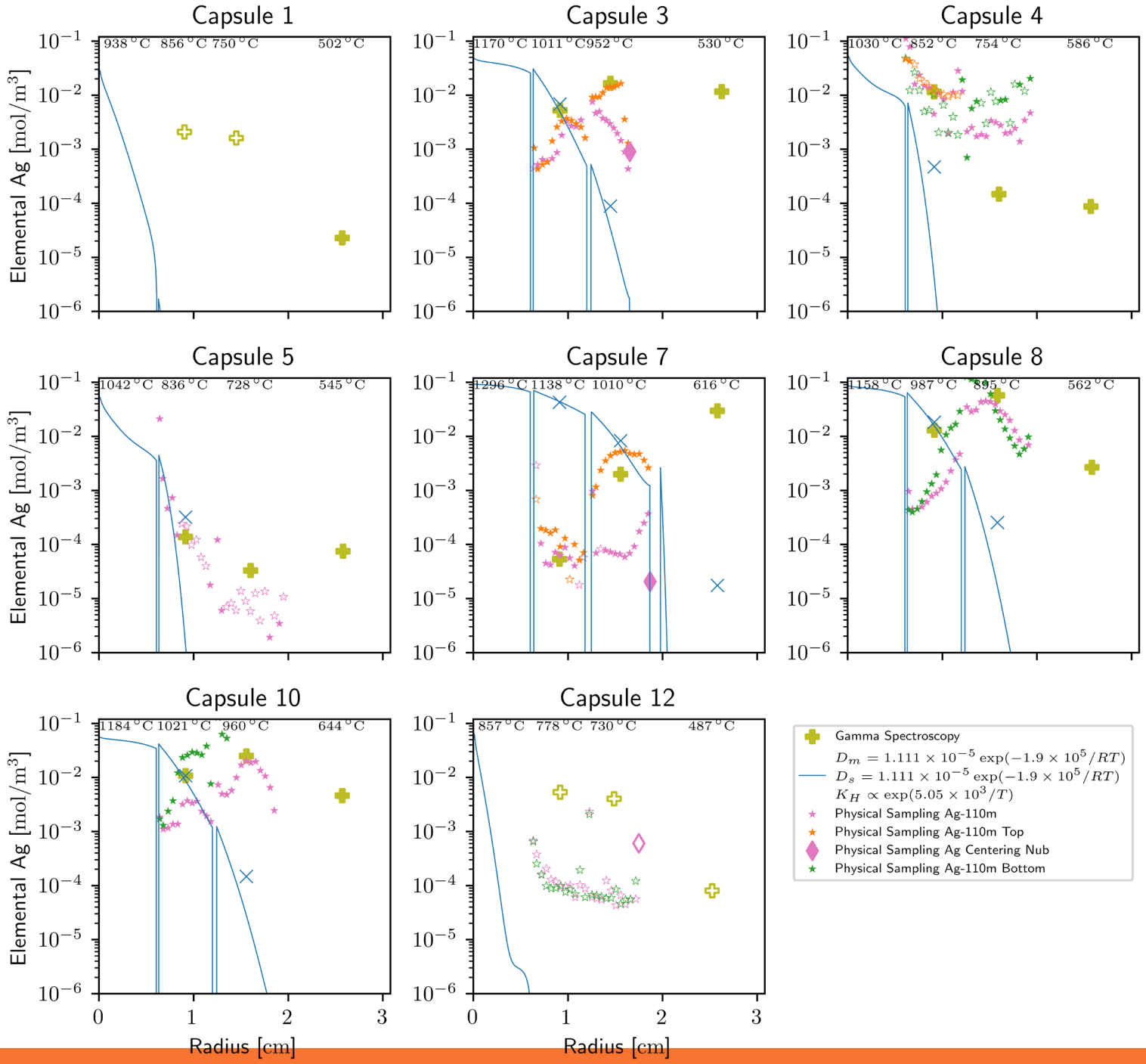




Next steps

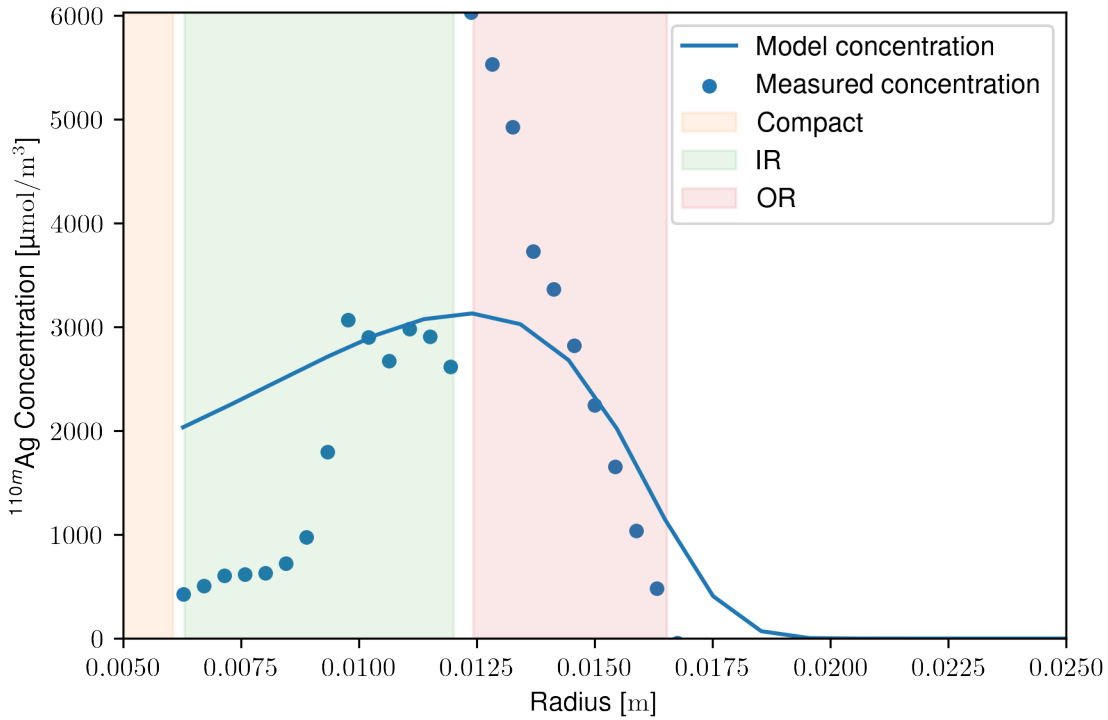
- Two mobile species
  - C_{bulk}, C_{fast}
  - $\frac{\partial C_{fast}}{\partial t} = D_{fast}\nabla^2 C_{fast} - k_A C_{fast} + k_f C_{bulk}$
  - $\frac{\partial C_{bulk}}{\partial t} = D_{bulk}\nabla^2 C_{bulk} + k_A C_{fast} - k_f C_{bulk}$
  - $k_f = \frac{k_A}{V_{fast} - C_{fast}}$
  - $D_{fast} = 10^4 D_{bulk}$
  - $D_{bulk} = D_0 \exp\left(-\frac{E_a}{RT}\right)$
  - Fit to find maximum fast transport volume V_{fast}, k_A, D_0, E_a

Silver


Capsule 1
938 °C 856 °C 750 °C 502 °C
Capsule 3
1170 °C 1011 °C 952 °C 530 °C
Capsule 4
1030 °C 852 °C 754 °C 586 °C
Capsule 5
1042 °C 836 °C 728 °C 545 °C
Capsule 7
1296 °C 1138 °C 1010 °C 616 °C
Capsule 8
1158 °C 987 °C 895 °C 562 °C
Capsule 10
1184 °C 1021 °C 960 °C 644 °C
Capsule 12
857 °C 778 °C 730 °C 487 °C
Elemental Ag [mol/m^3]
Radius [cm]
Gamma Spectroscopy
$D_m = 1.111 \times 10^{-5} \exp(-1.9 \times 10^5 / RT)$
$D_s = 1.111 \times 10^{-5} \exp(-1.9 \times 10^5 / RT)$
$K_H \propto \exp(5.05 \times 10^3 / T)$
Physical Sampling Ag-110m
Physical Sampling Ag-110m Top
Physical Sampling Ag Centering Nub
Physical Sampling Ag-110m Bottom

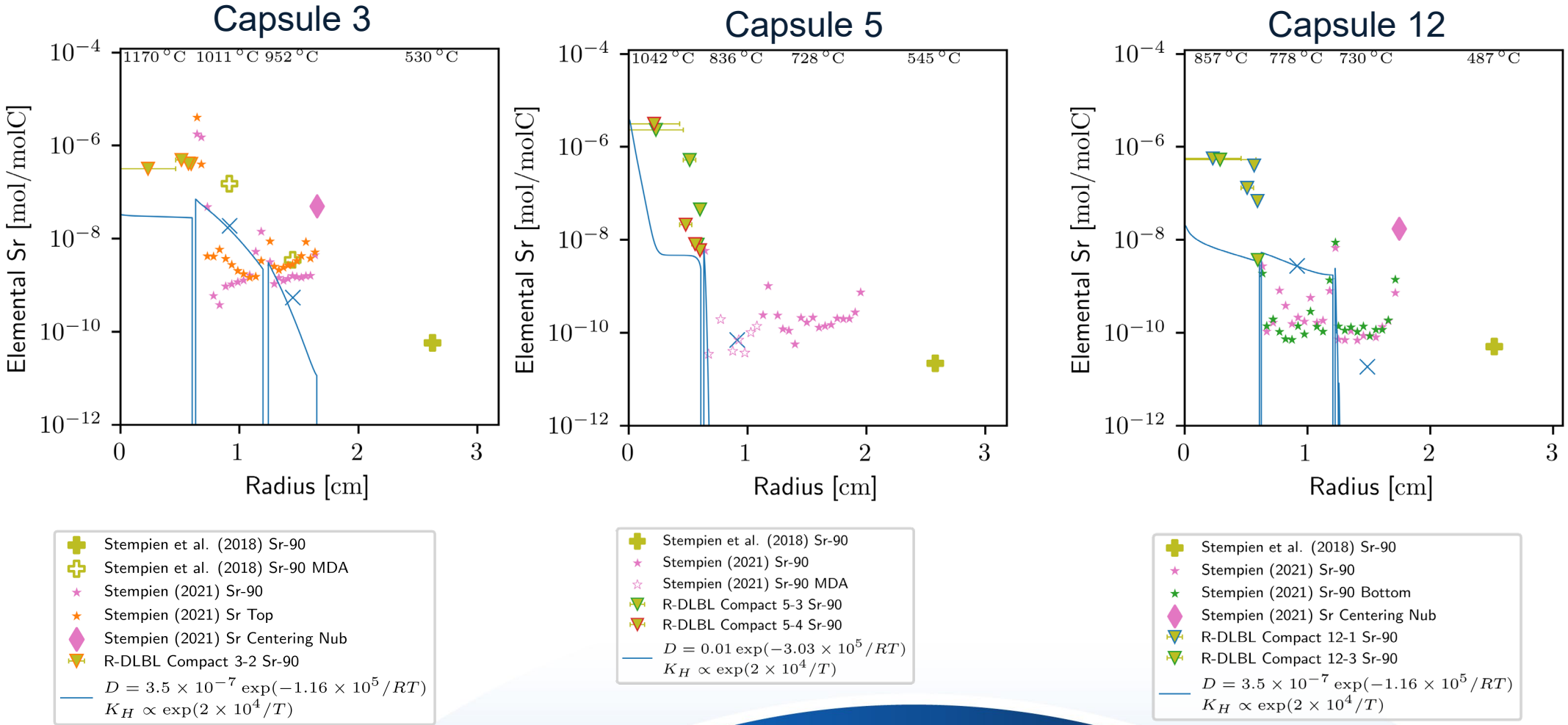
Silver Trapping Model best fit

- Preliminary trapping model
  - $\frac{\partial C_t}{\partial t} = k_t C_{bulk} - k_r C_t$
  - No upper limit to trap concentration
  - Able to demonstrate “bell-shaped” concentration profiles
  - Initial model ignores gaps between rings – fit parameters will change

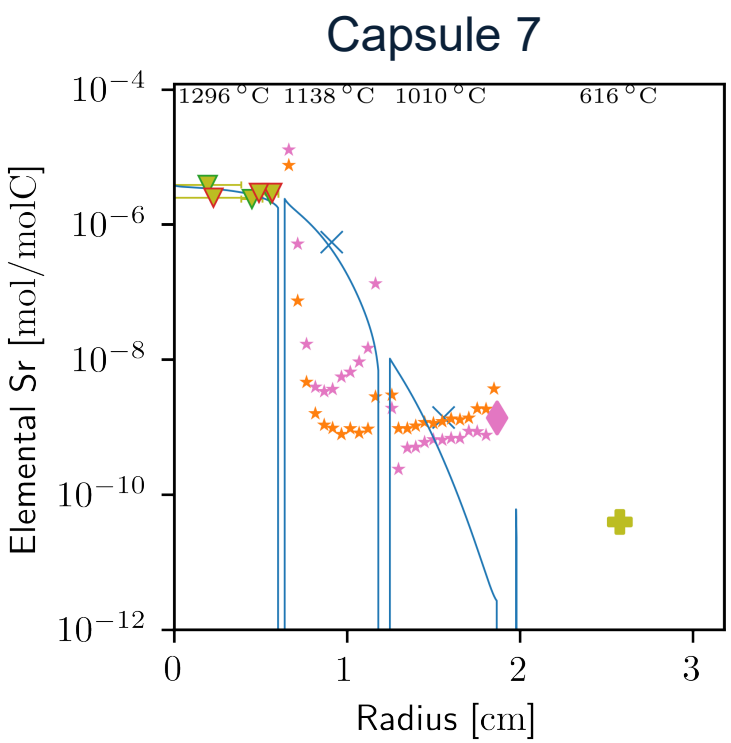


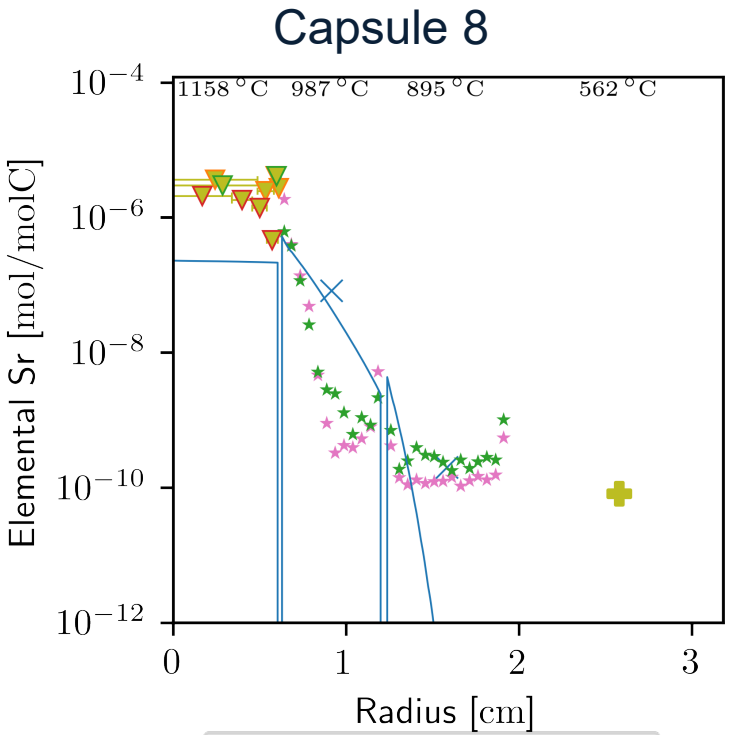
Strontium

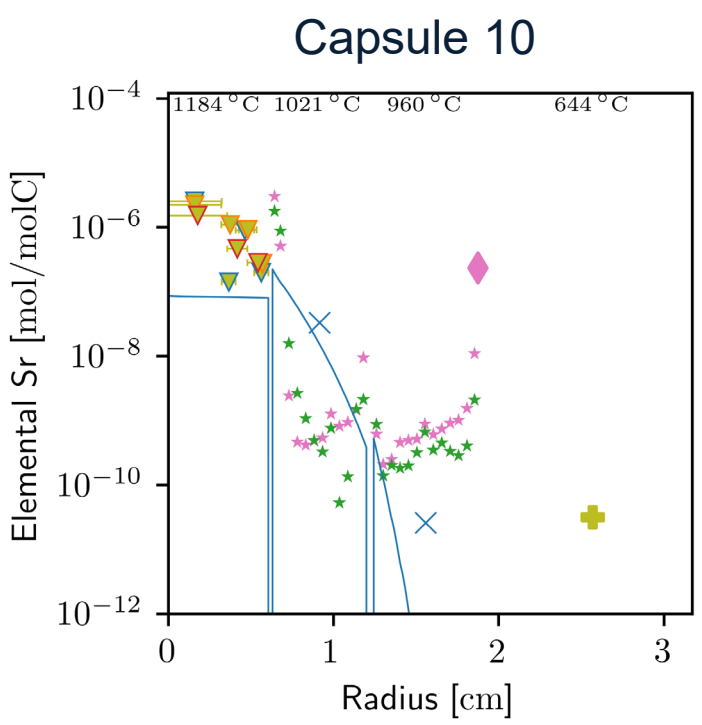
Capsule 3, 5, 12



Capsule 7, 8, 10







Strontium recap

- Likely to benefit from the dual mobility mechanism model
- DTF/Driver release rate may not be accurately estimated
- Concentration increases on outside of rings still unexplained

GAS-COOLED REACTOR

ADVANCED REACTOR TECHNOLOGIES PROGRAM

Thank You. Questions?

Adriaan Riet

Adriaan.riet@inl.gov

U.S. DEPARTMENT OF ENERGY