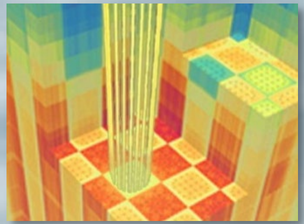
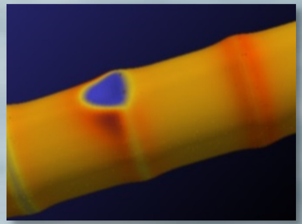
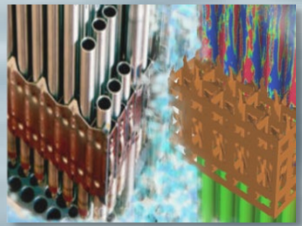
MAMBA
3D Pin-Wise CRUD Growth

VERA Workshop

February 11, 2019

VERA Users Group Meeting

Oak Ridge National Laboratory

The Consortium for Advanced Simulation of LWRs
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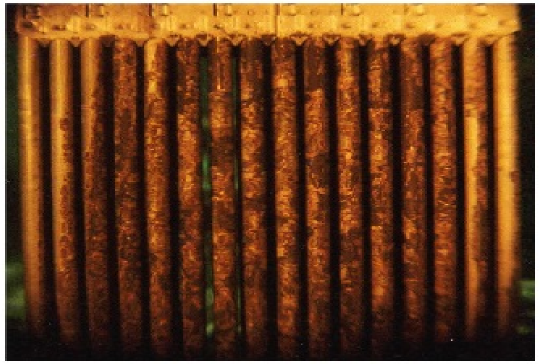
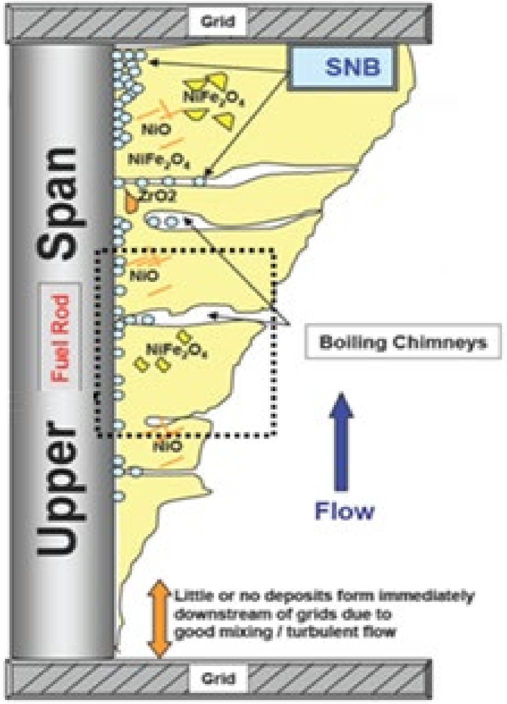
U.S. DEPARTMENT OF ENERGY

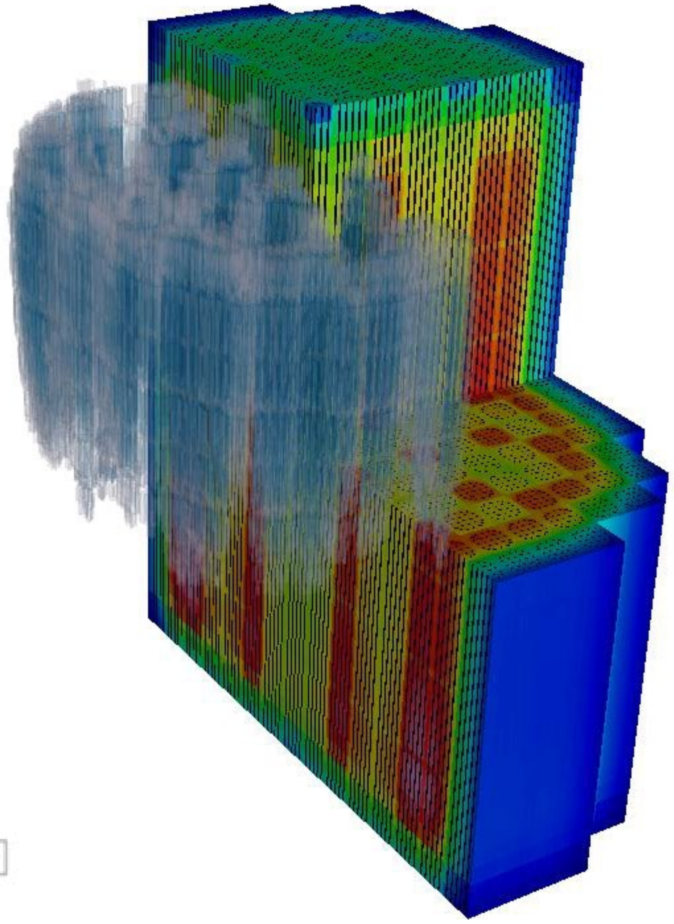
MAMBA: Advanced 3D Chemistry & CRUD

- Surface chemistry modeling of CRUD
- Microstructural chemistry and heat transfer
- Boron uptake and dissolution in the CRUD layer
- CFD-Informed Subchannel
  - Mapping of CFD to CTF for resolved flow
  - High-resolution prediction of threshold physics
- Source-terms
  - Metal ion pickup throughout primary loop
  - Calibration based on plant measurements
- Fully integrated in VERA for direct effect on power distributions





EPRI ELECTRIC POWER RESEARCH INSTITUTE

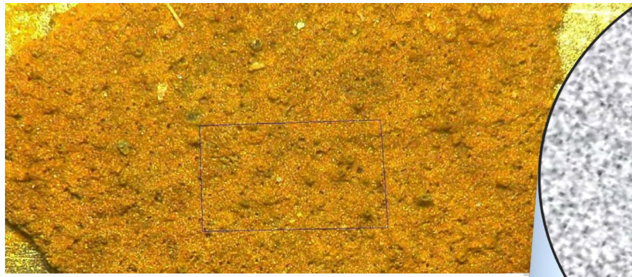


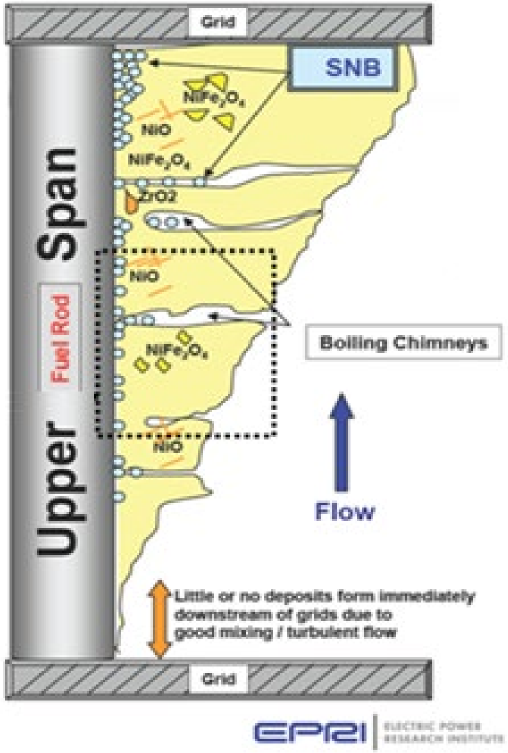
Simulated CRUD buildup

In Watts Bar 1 Cycle 7

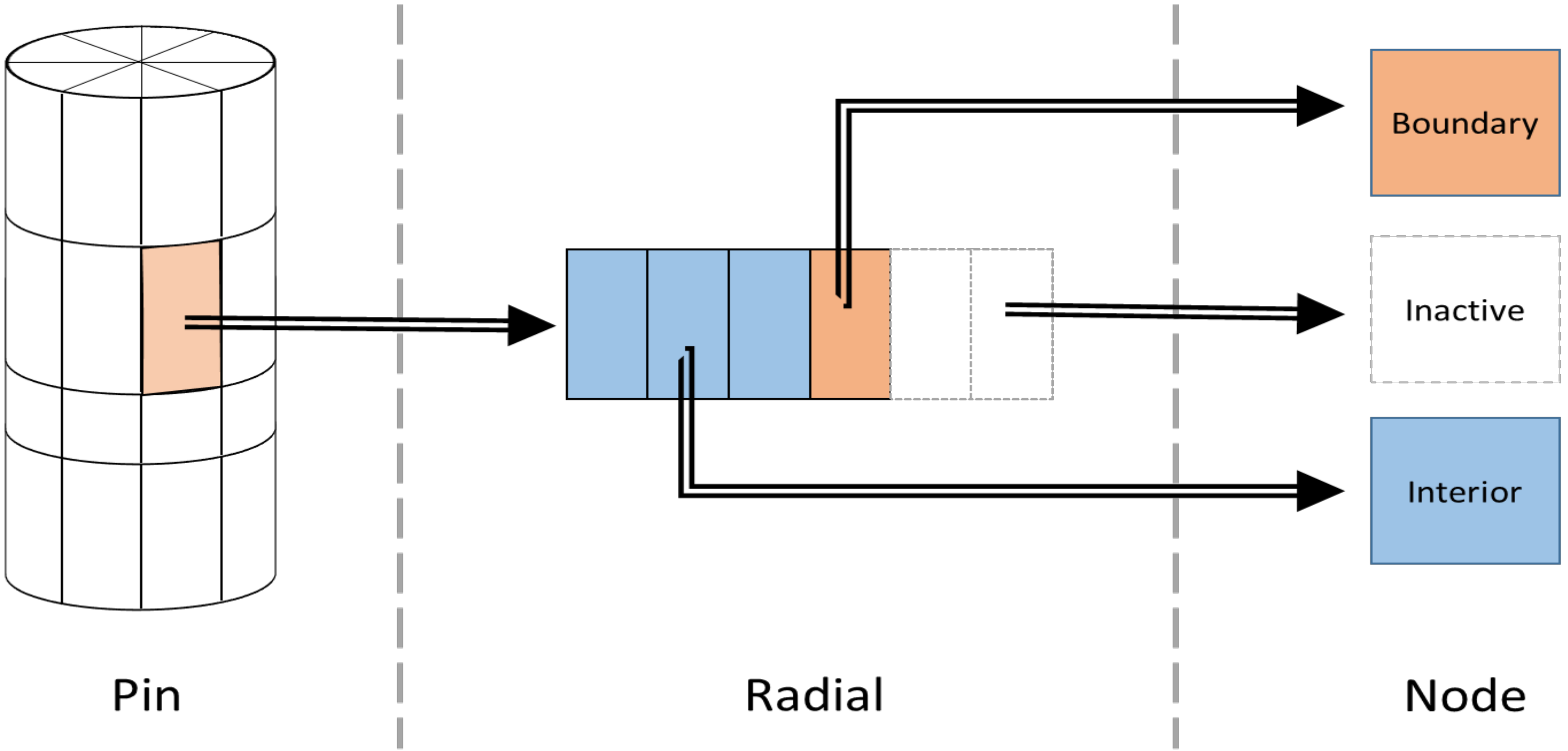
MAMBA: Conceptual Model

- Crud is a porous structure with chimneys
  - Focus on a single unit cell with chimney surrounded by porous structure
- Mechanics
  - Coolant water flows into porous structure and carries along soluble components in water
  - Particulates from water deposit on surface growing crud layer
  - Water boils inside the crud layer and vapor escapes through chimney
  - Boiling water leaves soluble components behind
  - With sufficient concentration soluble components precipitate out





MAMBA Conceptual Design



Coolant Thermodynamics

- Several soluble and solid phase species
  - Borate species – $B(OH)_3, B(OH)_4^-, B_2O(OH)_5^-, B_3O_3(OH)_4^-$
  - Lithium species – $LiOH, Li^+$
  - Water and hydrogen dissolution species – H_2O, OH^-, H^+, H_2
  - Iron ionic species – $Fe^{2+}, Fe(OH)_2$
  - Nickel ionic species – $Ni^{2+}, Ni(OH)_2$
  - Solid species – $NiFe_2O_4, Li_2B_4O_7$
- Solve borate, lithium, and hydrogen equilibrium first
- Use solution to determine iron and nickel including nickel ferrite precipitation parameter
- Lastly determine lithium tetraborate precipitation parameter

Surface Kinetics

- Crud surface is only nickel ferrite growth

Time rate change	Non-boiling deposition rate	Boiling deposition rate	Errosion rate

$$\frac{dC_{NiFe_2O_4}}{dt} = \left(k^p_{s,non-boil} + k^p_{s,boil} q''_{s,boil}\right) C^p_{NiFe_2O_4,cool} - \gamma_{s,e} k_{TKE}.$$

- $q_{s,boil}$ modified to include surface boiling by CTF and chimney boiling (enhances crud growth on "clean" surfaces)
- Analytic solution to the ODE describes the growth of the crud
- Crud is grown at a fixed porosity (70%) until a node is full

Internal Kinetics

- Nickel ferrite forms if concentration of Ni and Fe are sufficiently high

$$\frac{dC_{NiFe_2O_4}}{dt} = \begin{cases} k_i\eta\left(C_{Ni_s}C_{Fe_s}^2 - p_{NiFe_2O_4}C_{cool}^3\right) & C_{Ni_s}C_{Fe_s}^2 > p_{NiFe_2O_4}C_{cool}^3, \\ 0 & \end{cases}$$

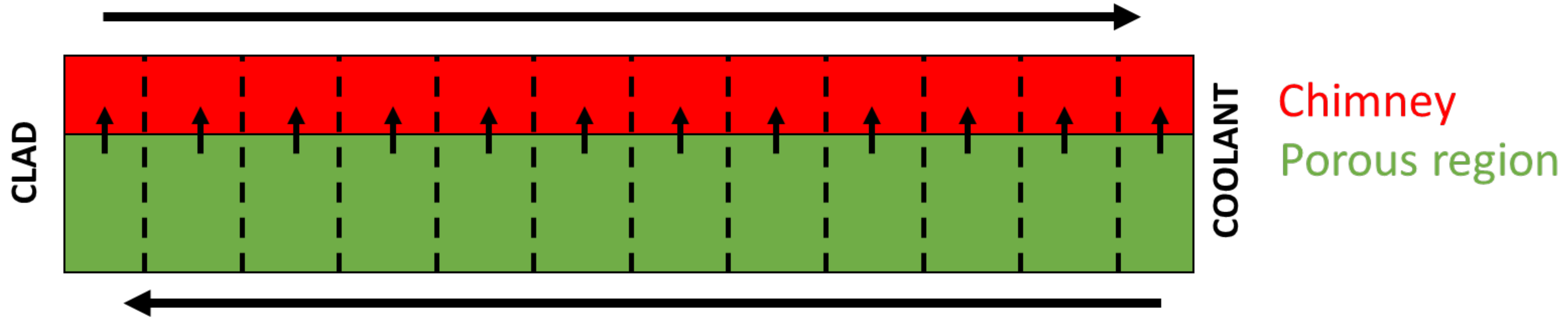
- Porosity, η, changes with $NiFe_2O_4$

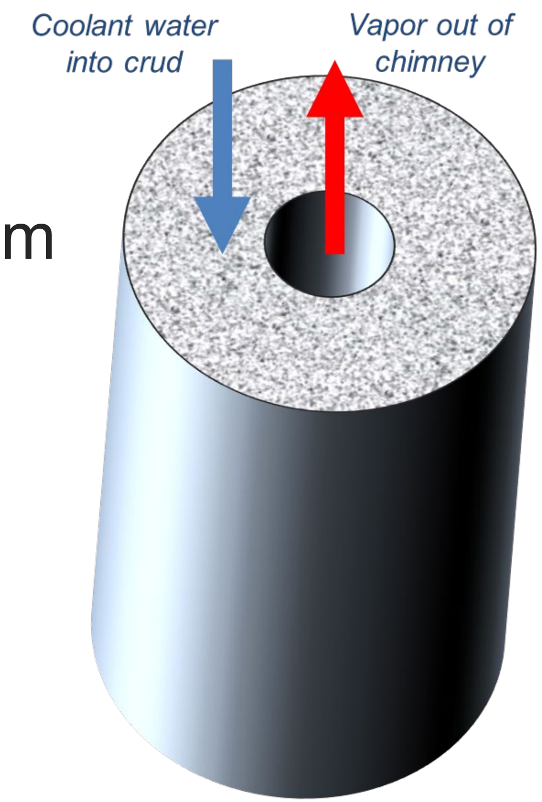
$$\frac{d\eta}{dt} = -\frac{M_{NiFe_2O_4}}{\rho_{NiFe_2O_4}}\frac{dC_{NiFe_2O_4}}{dt}.$$

- Similar form for Ni, NiO, Magnetite, and Bonaccordite has recently been implemented

MAMBA Internal Kinetics

- Mechanistic species transport model is developed which captures the convection and diffusion through the porous crud structure
  - Species convects in through the porous region
  - Concentration is increased through coolant boiling into the chimney
  - Species diffuses back out to the coolant
  - Included liquid carryover fraction in chimney region
- Lithium tetraborate is handled after the fact by checking lithium and boron concentrations: $C_B^4 C_{Li}^2 > p_{Li_2B_4O_7} C_{cool}^6,$
  - If precipitation occurs, the remaining porosity is filled to 99%





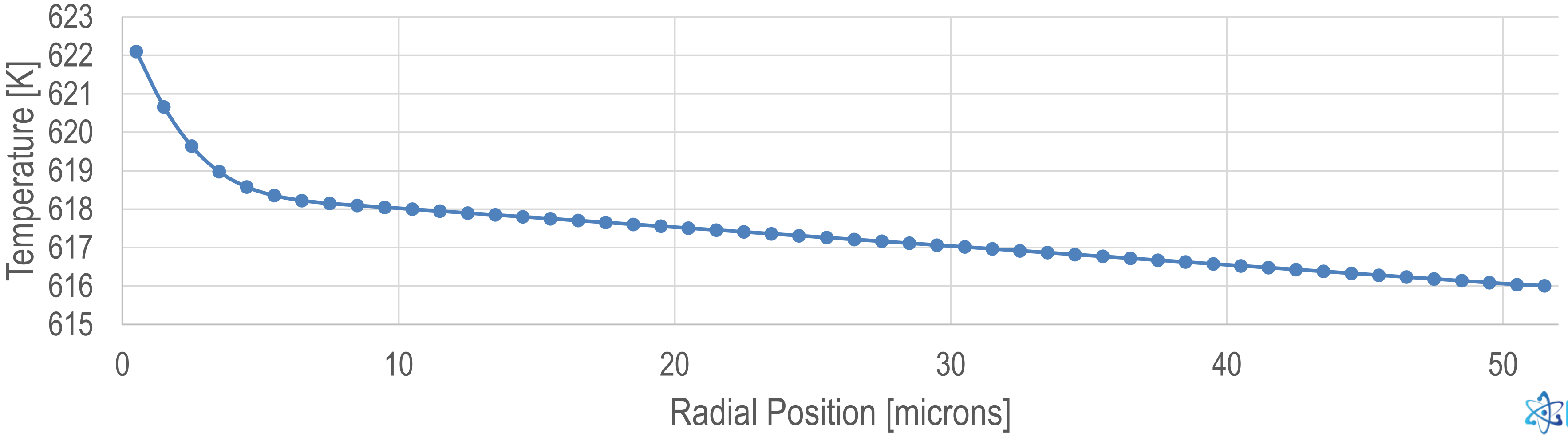
Heat conduction

- Heat conduction in the crud is driven by the significant heat sink caused by boiling

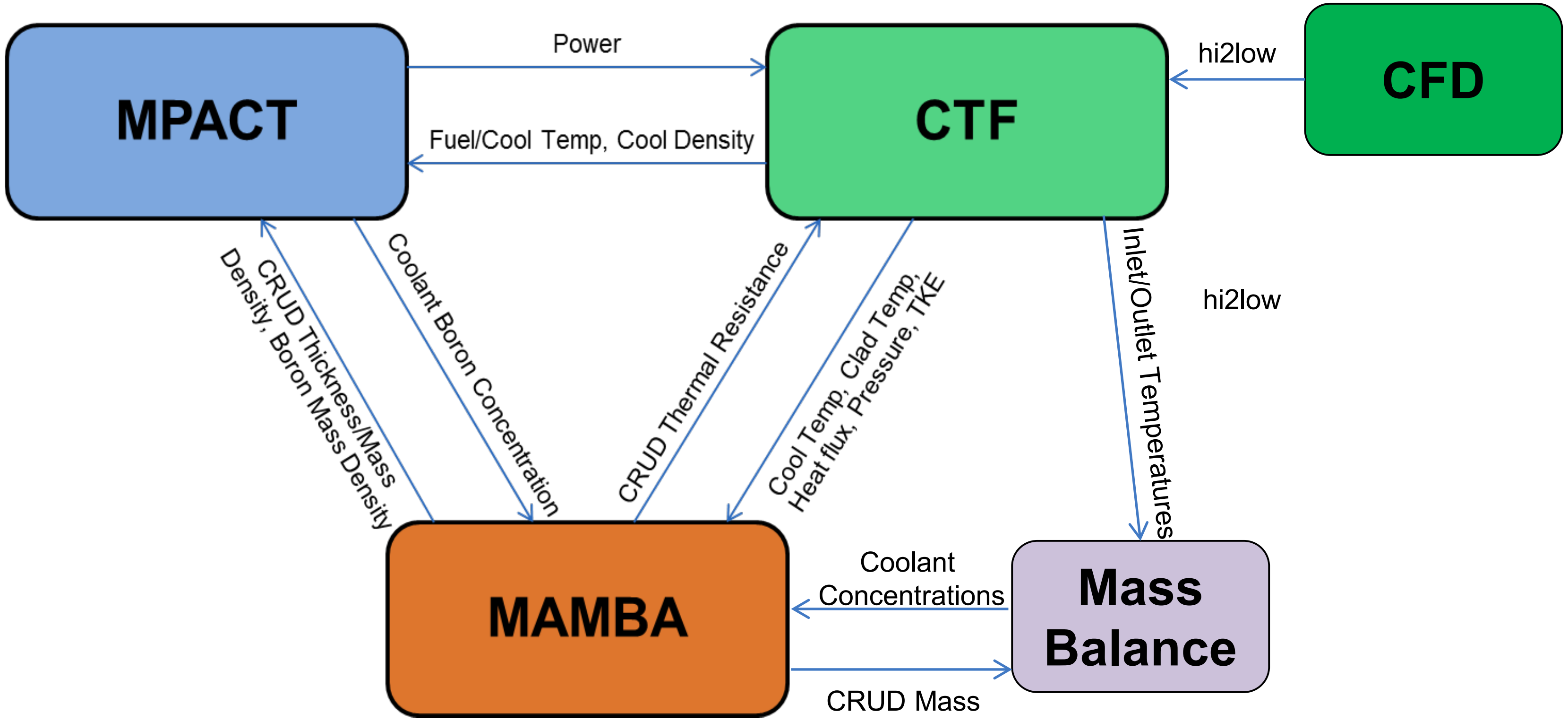
$$\nabla \cdot k\nabla \mathrm{T} = \mathrm{q}_{\mathrm{sink}}^{'''},$$

$$\mathrm{q}_{\mathrm{sink}}^{'''} = \begin{cases} 2\pi r_{chim}\mu(\eta)\, h_{chim}\rho_{chim}(T - T_{sat}) & T > T_{sat} \\ 0 & \end{cases},$$

- Current implementation is a steady-state, 1D model for every axial and azimuthal region



Modeling CRUD requires tight coupling to other components of VERA



Single capability to handle CIPS and CILC

Improvements to VERA for CRUD Simulations

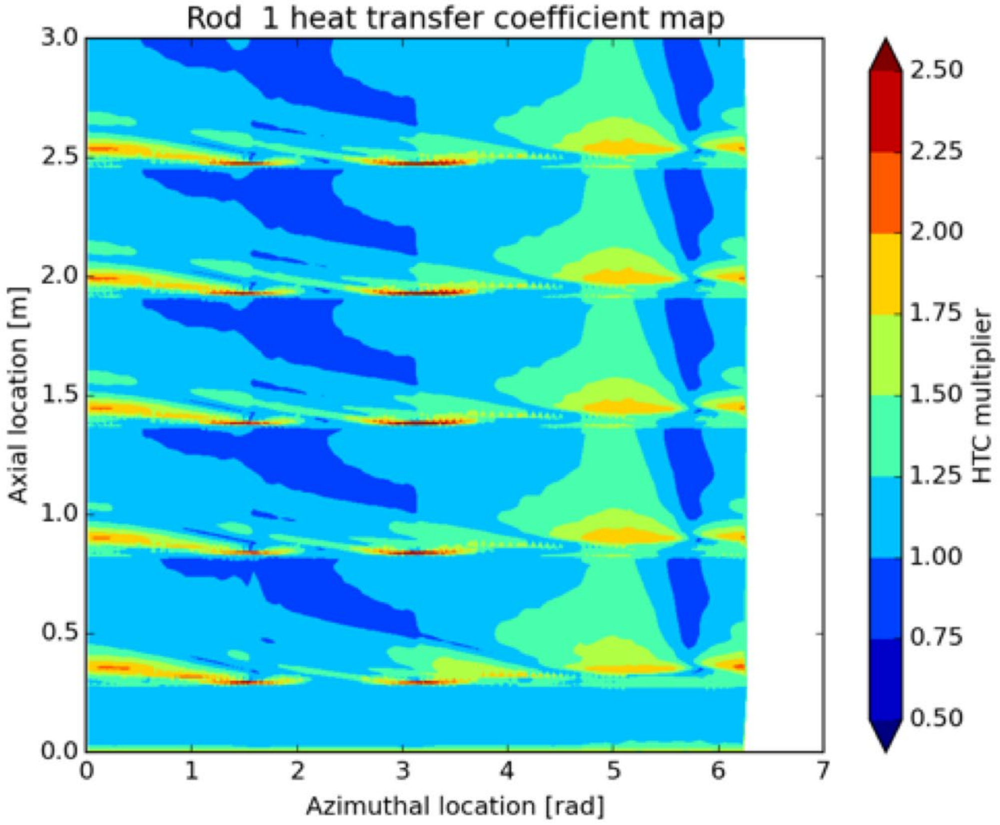
- Multicycle capability
  - Shuffle CRUD built in on previous assemblies
  - Remove CRUD due to thermal/mechanical/chemical shock and ultrasonic cleaning
- Improved coupling
  - Boron-10 depletion in CRUD layer
  - Better model for energy balance at CRUD-Coolant interface
- Improve mass balance
  - User specified alloy, surface area, etc. for steam generator and piping
  - Simplified Lithium program input

ROTHCON: Improving Resolution with CFD Data

- Develop heat transfer and turbulent kinetic energy multiplier maps as function of rod surface location and grid geometry
- Add capability in CTF to create a refined coupling mesh for MAMBA coupling

$$M(z - z_g, \theta) = \frac{Nu_{grid}(z - z_g, \theta)}{Nu_{bare}(z - z_g)}$$

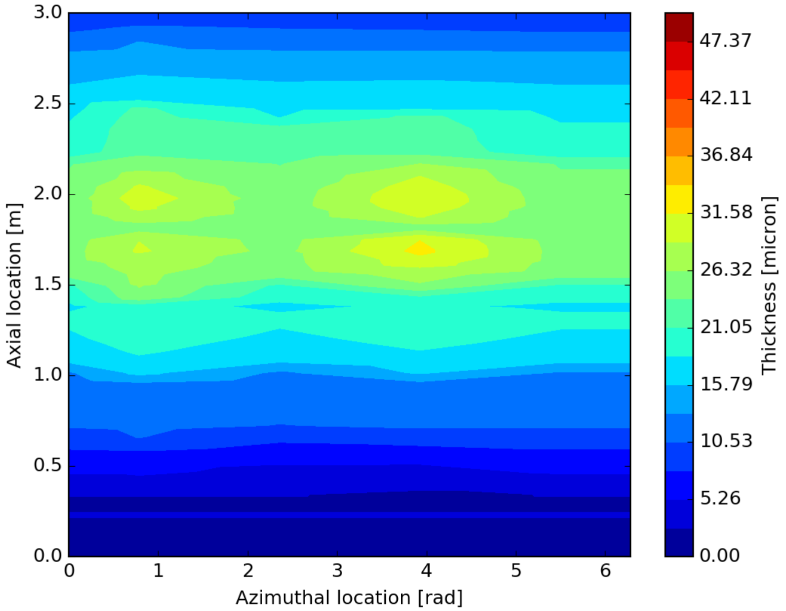
- Develop CFD models to generate data for reconstruction



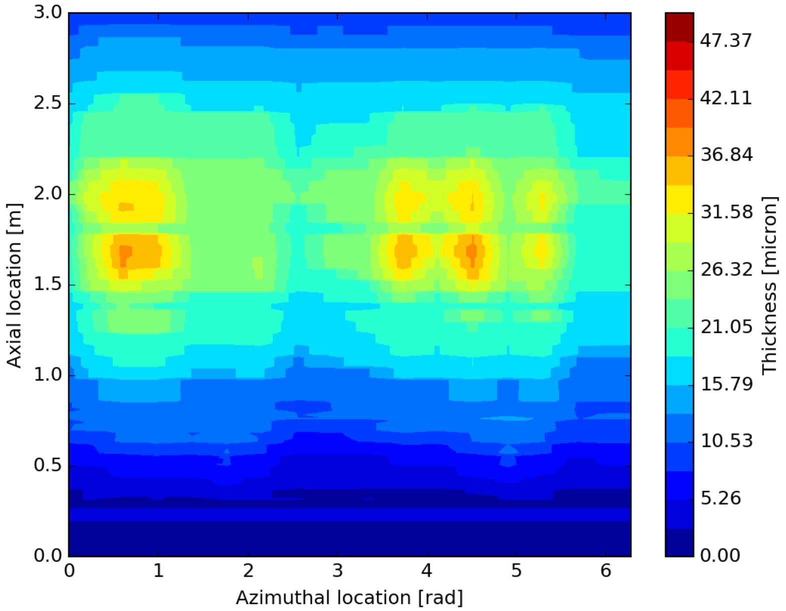
Example of HTC rod surface data map developed by STAR-CCM+ and read by CTF

Crud/Corrosion ROTHCON sensitivity

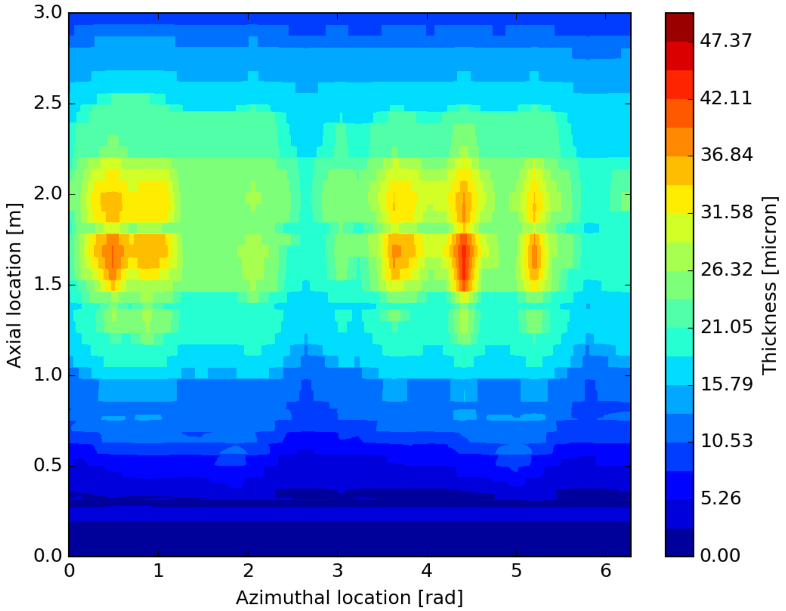
- Localized corrosion becomes thicker for higher levels of coupling mesh refinement
- Rod 22 surface corrosion behavior shown for different refinement levels



1x1 mesh refinement

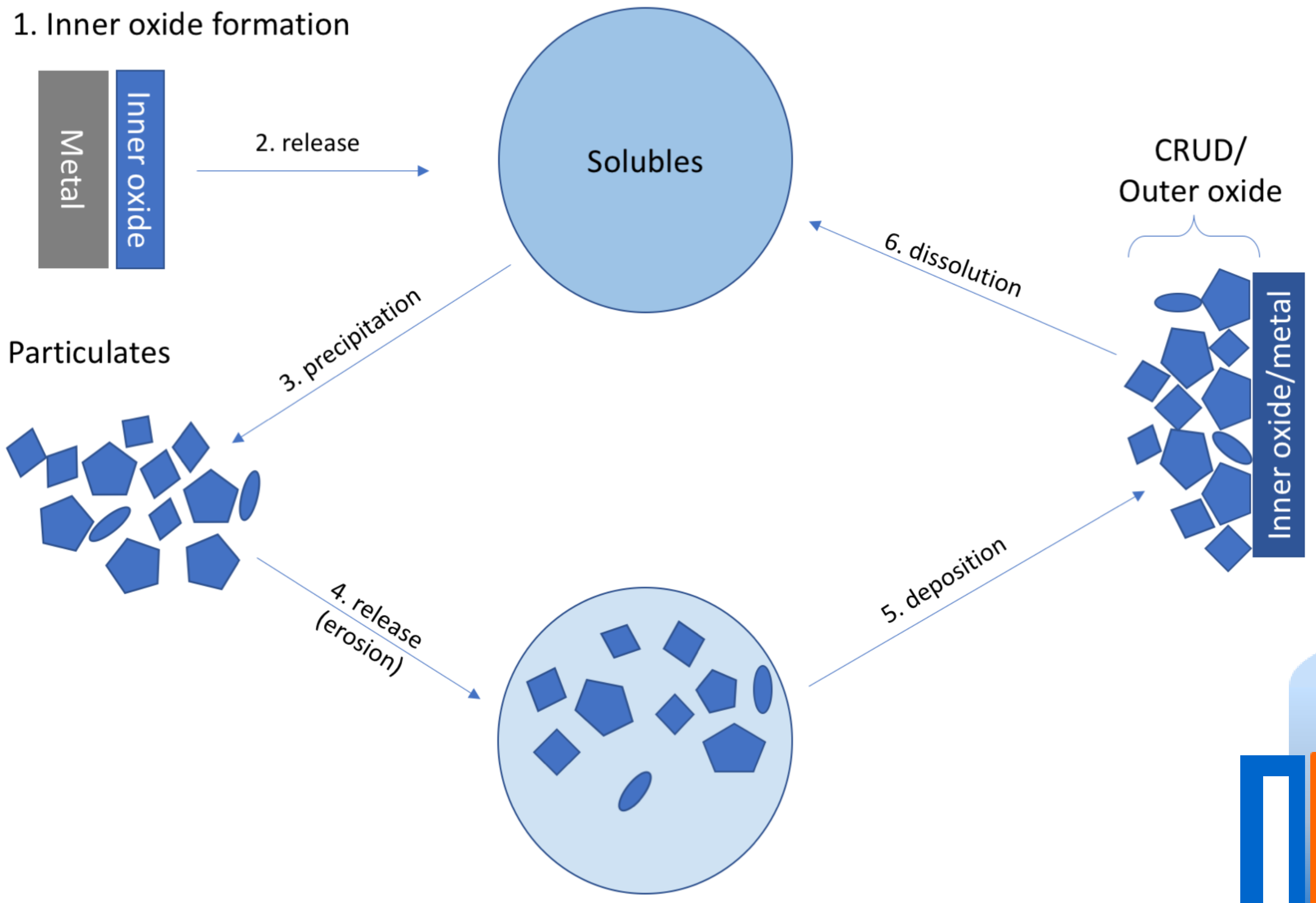


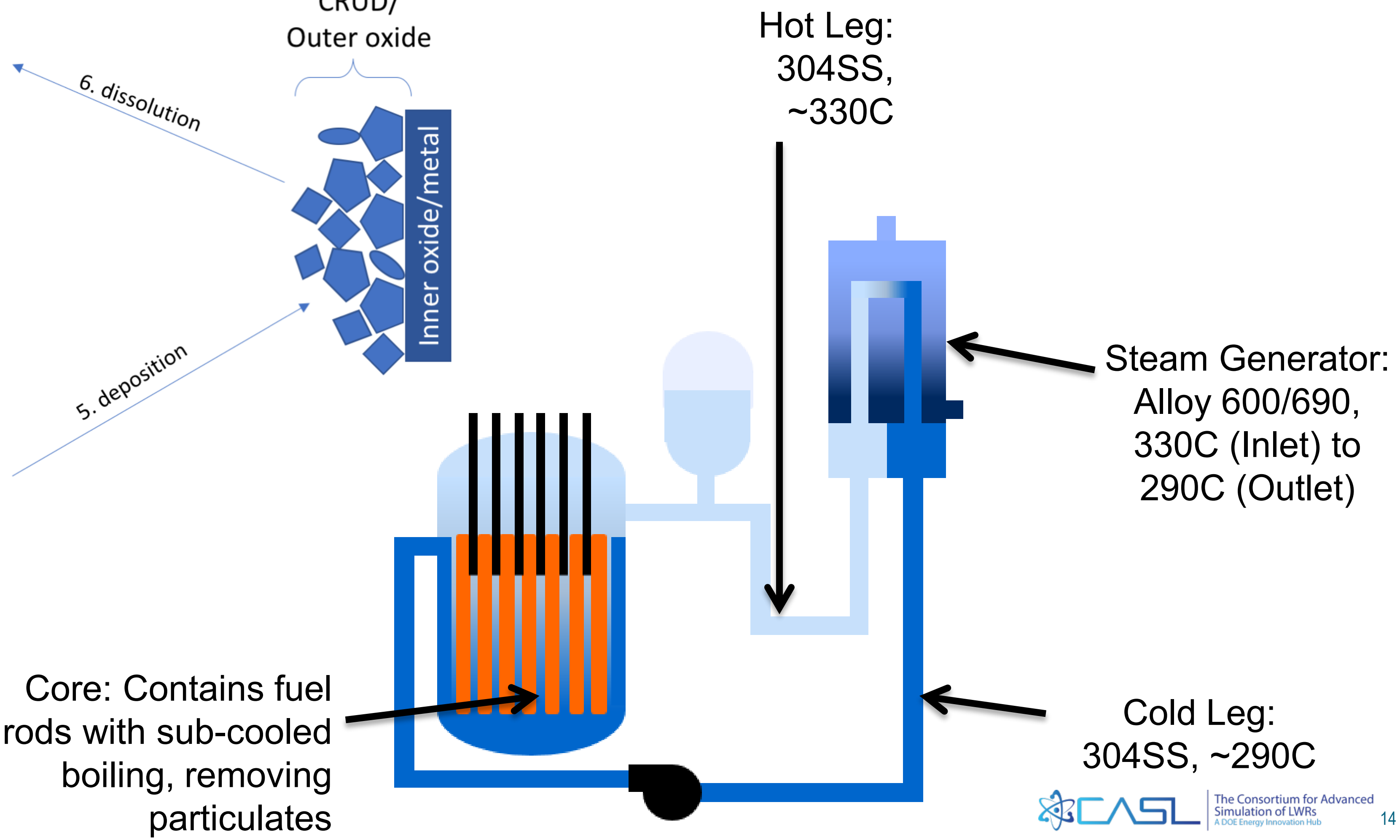
4x4 mesh refinement



8x8 mesh refinement

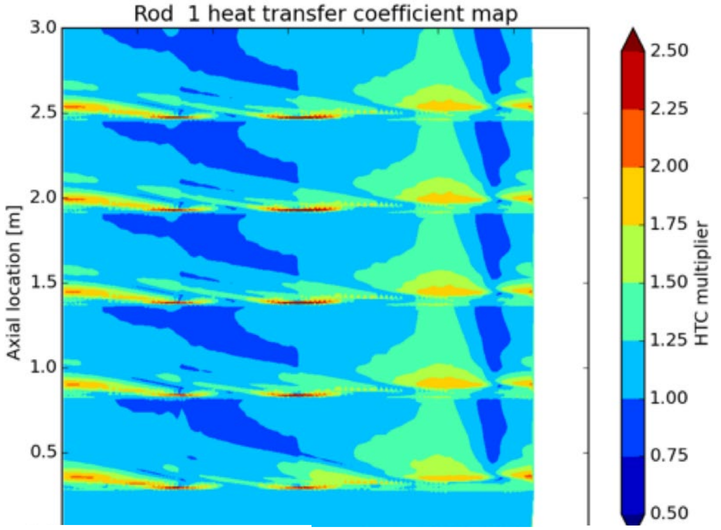
System mass balance model improves crud deposition models

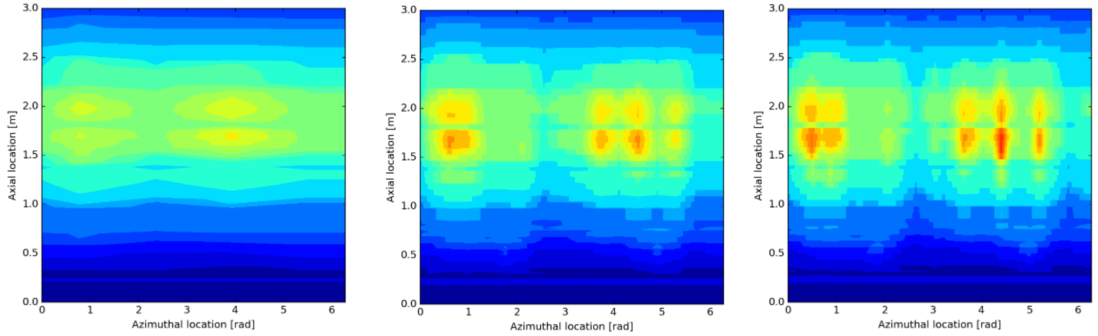




CILC screening capability demonstration

- CILC screening tool using MAMBA, CTF informed by STAR-CCM+, and clad/oxidation model

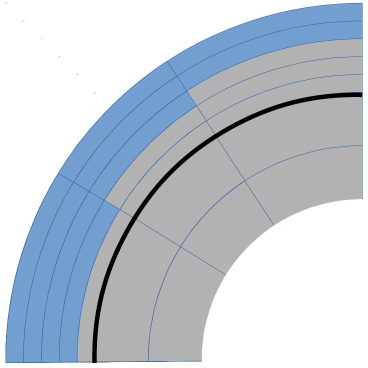




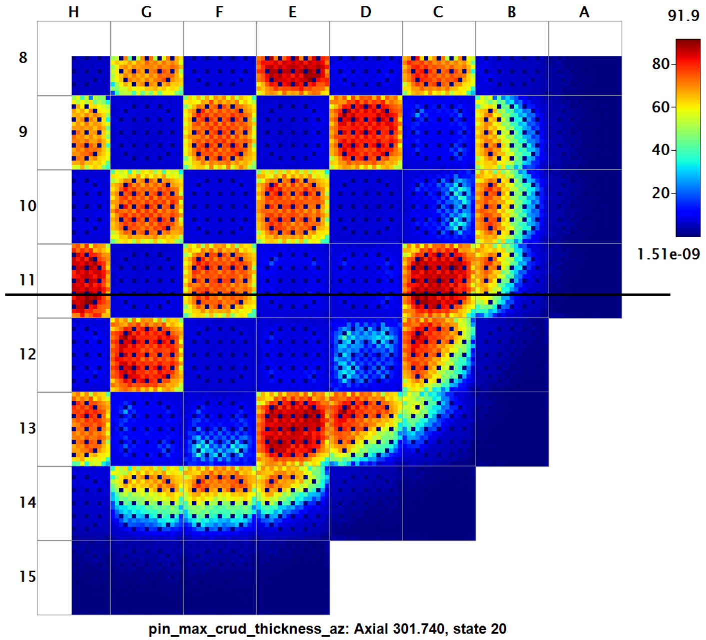
1x1 mesh 4x4 mesh 8x8 mesh

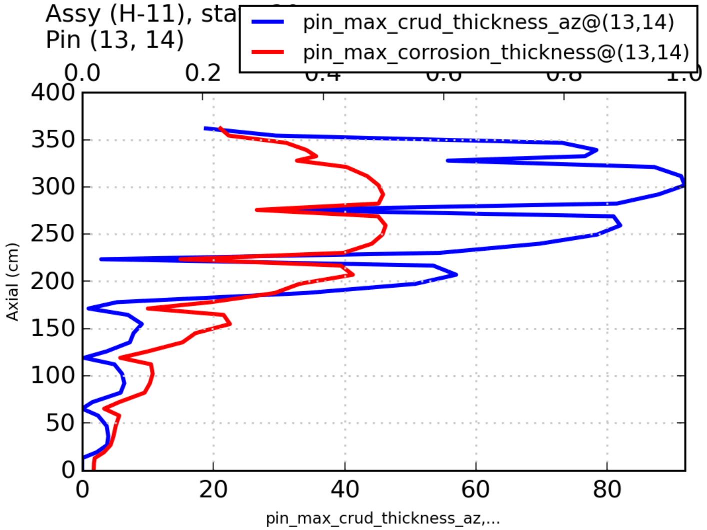
ROTHCON method reconstructs Star-CCM+ solution onto CTF mesh

Oxidation model integrated with CTF



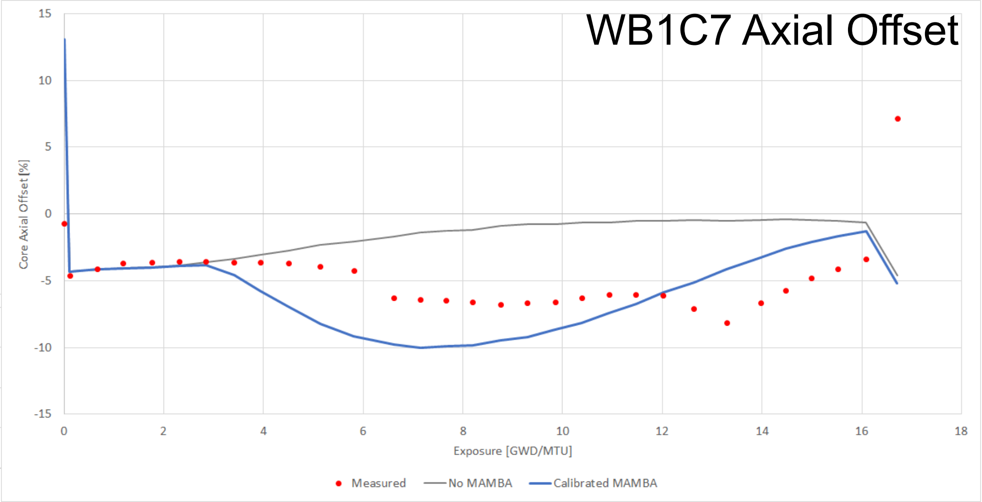
Seabrook Cycle 5 Demonstration

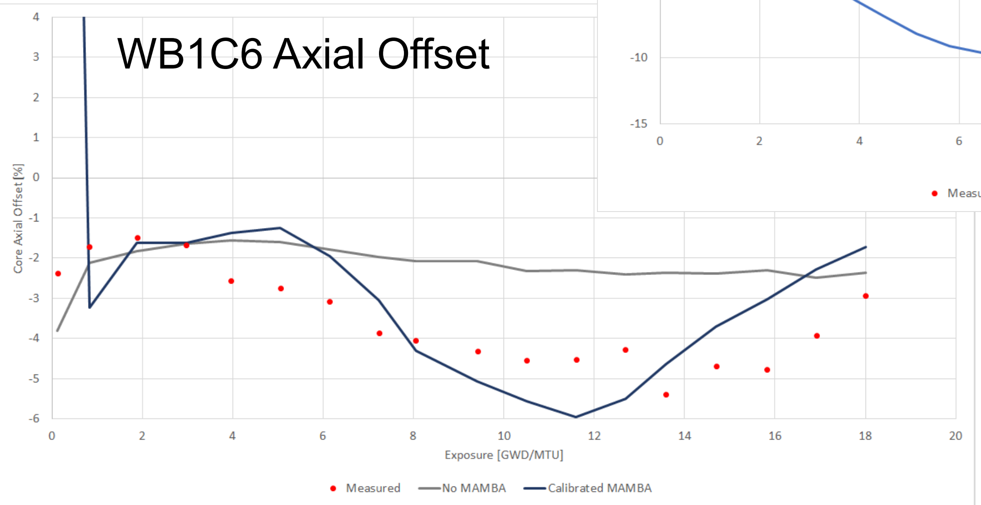


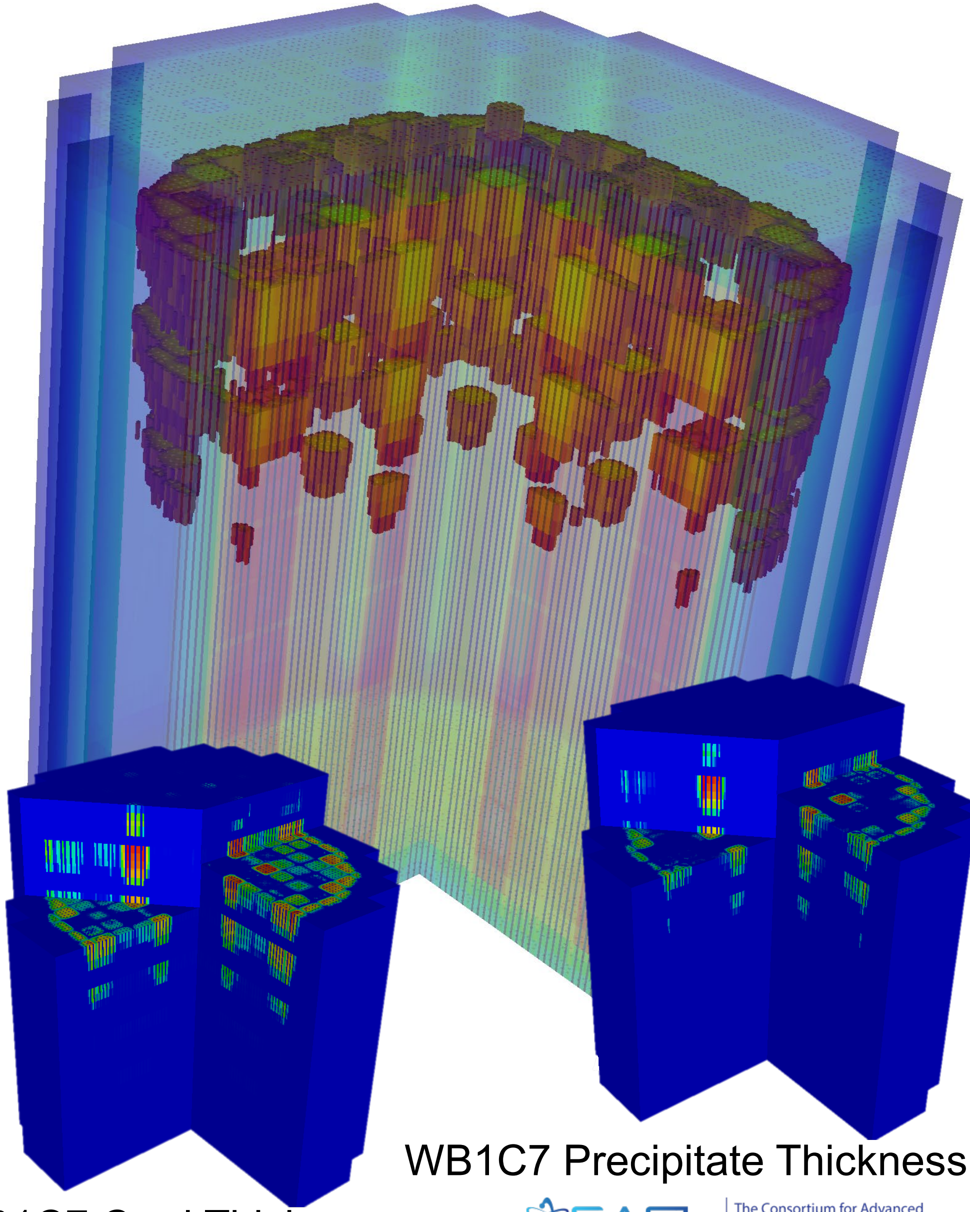


CIPS simulation capability for Watts Bar Unit 1 Cycle 6 and 7

- CIPS hand calibration for WB1C7 and the application of calibrated parameters for WB1C6



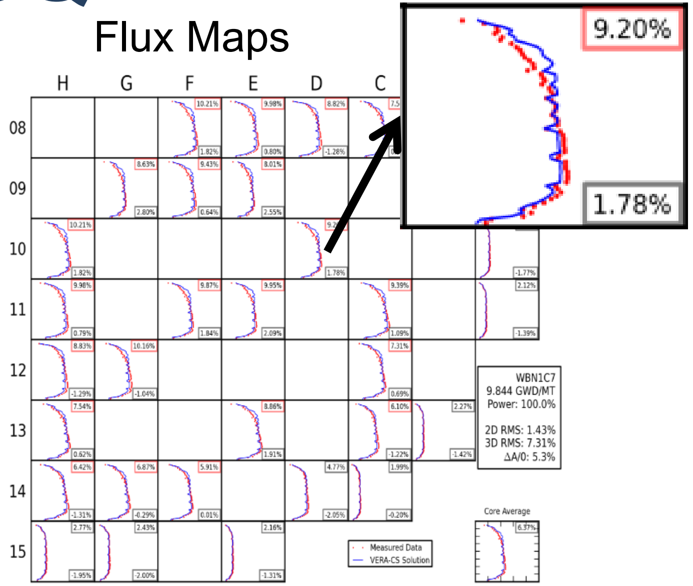




Path towards CRUD predictions with UQ Calibration with uncertainty

Watts Bar	Catabwa	Vogtle
$\gamma_{src,wb}$	$\gamma_{src,c}$	$\gamma_{src,v}$
Cycle 4	Cycle 7	Cycle 9
5	**8**	**10**
6	9	11
7	10	12

Flux Maps

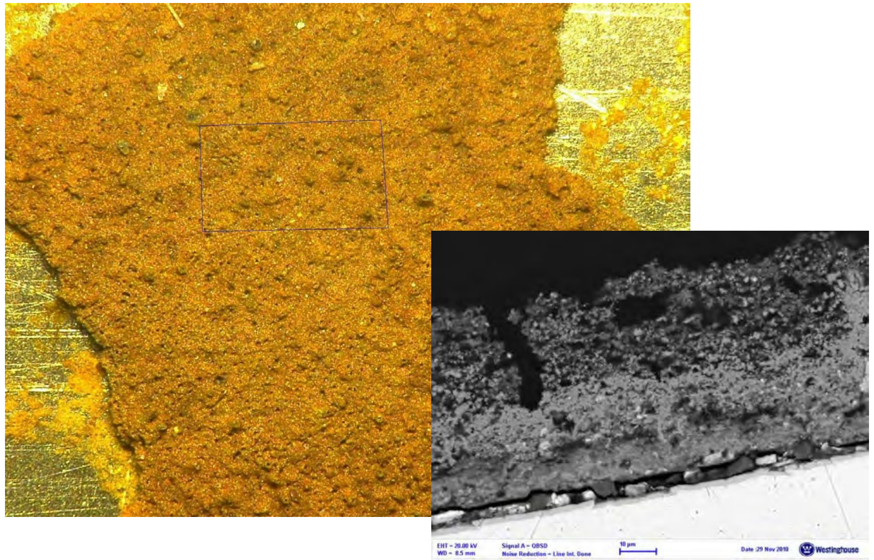


MAMBA

k_{snb} h_{boil} $A_{NiFe_2O_4,in}$ α_{chim} ....

Walt Loop

- Bayesian calibration will be performed with all available data
- Joint milestones with VVI, FMC, PHI, and AMA to calibrate CRUD capability



CRUD Scrapes

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