Crud Development and Calibration

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CASL Industry Council
April 23, 2019

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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

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 Model Development

Coolant water into crud

Vapor out of chimney
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

\[
\frac{dC_{NiFe_2O_4}}{dt} = \left(k_{s,\text{non-boil}}^{p} + k_{s,\text{boil}}^{p} q_s^{"}\right) C_{NiFe_2O_4,cool}^{p} - \gamma_s e^{k_{TKE}}.
\]

- \( q_s^{\text{boil}} \) 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 until a node is full
Internal Chemical Kinetics

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

\[
\frac{dC_{\text{NiFe}_2\text{O}_4}}{dt} = \begin{cases} 
    k_i \eta \left( C_{\text{Ni}_s} C_{\text{Fe}_s}^2 - p_{\text{NiFe}_2\text{O}_4} C_{\text{cool}}^3 \right) & \text{if } C_{\text{Ni}_s} C_{\text{Fe}_s}^2 > p_{\text{NiFe}_2\text{O}_4} C_{\text{cool}}^3 \\
    0 & \text{otherwise}
\end{cases}
\]

• Similar form for Ni and Bonaccordite
• Porosity, \( \eta \), changes

\[
\frac{d\eta}{dt} = -\frac{1}{\rho_{\text{crud}}} \left( M_{\text{NiFe}_2\text{O}_4} \frac{dC_{\text{NiFe}_2\text{O}_4}}{dt} + M_{\text{Ni}} \frac{dC_{\text{Ni}}}{dt} + M_{\text{Ni}_2\text{FeBO}_5} \frac{dC_{\text{Ni}_2\text{FeBO}_5}}{dt} \right)
\]
MAMBA has the ability to simulate multiple solid chemical compositions found in crud scrapes

Important species:
- Nickel metal (Ni)
- Nickel ferrite (NiFe$_2$O$_4$)
- Bonaccordite (Ni$_2$FeBO$_5$)
- Lithium tetraborate (Li$_2$B$_4$O$_7$)

Thermodynamically favorable reactions:

• **Precipitation of nickel ferrite:**
  \[ 2\text{Fe}^{2+} + \text{Ni}^{2+} + 4\text{H}_2\text{O} \rightarrow \text{NiFe}_2\text{O}_4(s) + 6\text{H}^+ + \text{H}_2(g) \]

• **Precipitation of nickel metal:**
  \[ \text{Ni}^{2+} + \text{H}_2(g) \rightarrow \text{Ni}(s) + 2\text{H}^+ \]

• **Precipitation of bonaccordite:**
  - From soluble species
    \[ \text{Fe}^{2+} + 2\text{Ni}^{2+} + \text{B(OH)}_3 + 2\text{H}_2\text{O} \rightarrow \text{Ni}_2\text{FeBO}_5(s) + 6\text{H}^+ + 0.5\text{H}_2(g) \]
  - From nickel metal
    \[ 2\text{Ni}(s) + \text{Fe}^{2+} + \text{B(OH)}_3 + 2\text{H}_2\text{O} \rightarrow \text{Ni}_2\text{FeBO}_5(s) + 2\text{H}^+ + 2.5\text{H}_2(g) \]
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• **Precipitation of lithium tetraborate:**
  \[ 2\text{Li}^+ + 4\text{B(OH)}_3 \rightarrow \text{Li}_2\text{B}_4\text{O}_7(s) + 5\text{H}_2\text{O} + 2\text{H}^+ \]

Other notes:
Nickel metal (Ni) is more stable than nickel oxide (NiO) within the crud during reactor operation.
Nickel ferrite (NiFe$_2$O$_4$) is thermodynamically preferred over nickel metal (Ni).
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: $C_B^4C_{Li}^2 > P_{Li_2B_4O_7}C_{cool}^6$.
  - 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

\[ \nabla \cdot k \nabla T = q_{\text{sink}}, \]
\[ q_{\text{sink}} = \begin{cases} 
2\pi r_{\text{chim}} \mu(\eta) h_{\text{chim}} \rho_{\text{chim}} (T - T_{\text{sat}}) & T > T_{\text{sat}}, \\
0 & \text{otherwise} \end{cases} \]

• Current implementation is a steady-state, 1D model for every axial and azimuthal region
Modeling CRUD requires tight coupling to other components of VERA

- MPACT
  - Power
  - Fuel/Cool Temp, Cool Density
- CTF
  - CRUD Thermal Resistance
  - Cool Temp, Clad Temp, Heat flux, Pressure, TKE
- CFD
  - hi2low
- MAMBA
  - Coolant Concentrations
  - CRUD Mass
- Mass Balance
  - Inlet/Outlet Temperatures

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
  – Updated source term model
  – User specified alloy, surface area, etc. for steam generator and piping
  – Simplified Lithium program input
System mass balance model improves crud deposition models

1. Inner oxide formation
2. Release
3. Precipitation
4. Release (erosion)
5. Deposition
6. Dissolution

Solubles

CRUD/Outer oxide

Inner oxide/metal

Particulates

Hot Leg: 304SS, ~330C

Steam Generator: Alloy 600/690, 330C (Inlet) to 290C (Outlet)

Core: Contains fuel rods with sub-cooled boiling, removing particulates

Cold Leg: 304SS, ~290C

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Hot Leg: 304SS, ~330C
5 steps of crud “life cycle” should be present in a source term model

1. Base metal corrodes to form inner oxide layer
2. Ions diffuse from base metal to coolant through inner oxide (corrosion release)
3. Particulates form on inner oxide surface by precipitating from solubles to form outer oxide
4. Particulates enter coolant due to erosion of outer oxide/crud layer
5. Coolant particulates deposit on fuel as crud
2 steps are present in existing MAMBA; Coupling of solubles to particulates is not currently modeled
New model adds remaining 3 steps to the system mass balance
New model adds remaining 3 steps to the system mass balance

\[
\frac{dC_{Ni}}{dt} = \sum_{SG \text{ Area}} \left[ \frac{D_{Ni}(T_i) \rho_{alloy} \ wt\% (Ni)}{k_p(T_i) \sqrt{t}} \times A_i \right] - \frac{k_c}{n_{Ni}} (C_{Ni} - C_{Sat})
\]

2. Corrosion release

\[
\frac{dW}{dt} = \frac{k_c}{n_{Ni}} (C_{Ni} - C_{Sat}) - k_e W
\]

3. Precipitation

4. Release (erosion)

\[
\frac{dC_p}{dt} = k_e W - \dot{M} C_p + \dot{e}
\]

4. Release (erosion)

5. Net Core Crud deposition

\[
\frac{dC_{NiFe_2O_4}}{dt} = (k_{p,s,non-boil} + k_{p,s,boil} \dot{q}_{s,boil}''') C_{NiFe_2O_4,cool}^p - \gamma_{s,e} k_{TKE}
\]

\( \dot{M} \) and \( \dot{e} \) come from integrals over the core
Comparison of time stepping methods

<table>
<thead>
<tr>
<th>Case</th>
<th>Walltime [s]</th>
<th>$\Delta t$ [days]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Semi-Analytic</td>
<td>31.5</td>
<td>1.0</td>
</tr>
<tr>
<td>Implicit</td>
<td>199.3</td>
<td>1.0</td>
</tr>
<tr>
<td>Explicit</td>
<td>261.5</td>
<td>0.1</td>
</tr>
</tbody>
</table>
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
- Surface corrosion behavior shown for different refinement levels

1x1 mesh refinement

4x4 mesh refinement

8x8 mesh refinement
CRUD predictions with UQ
Calibration with uncertainty

Watts Bar 1
\( \gamma_{src,wb} \)
Cycle 5
6

Catabwa 1
\( \gamma_{src,c} \)
Cycle 7
8

Vogtle 1
\( \gamma_{src,v} \)
Cycle 9
10

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

MAMBA
\( k_{snb} \ h_{boil} \ A_{NiFe2O4.out} \ \alpha_{chim} \ \gamma_{erosion} \)

CRUD Scrapes

Flux Maps

9.20%
1.78%
Tasks

• WALT loop data calibration
  – Automate the calibration and forward propagation with Dakota doing the calibration
  – Need to extract the remaining rods data into data files
  – Demonstration of the plant level calibration/forward propagation.

• MPACT “surrogate” for boron to detector response
  – Use previous simulation data that provides the impact of boron on the detector signal
  – Using SciKit learn to build a surrogate

• Multicycle driver for MAMBA-only
  – Multicycle coupled steam generator crud precursor release model with core crud model
  – Parallelizable via MPI
  – Interoperable with standard VERA tools and input/output formats.

• Develop VERA runs and inputs for calibration cycles
  – All of the data needs to be gathered, models set up, and run once to ensure good comparison for non-CIPS cycles.
WALT Loop Calibration

- WALT loop provides thermal resistance measurements for variety of measured crud thicknesses and heat fluxes
- MAMBA is run for all rods in dataset provided and calibrated thermal conductivity, heat transfer coefficient, and chimney vapor fraction
- Bayesian calibration provides most probable values as well as a probability distribution for each parameter
- Mean + 3 sigma used in core calibration
Calibration Sequence

- Run coupled VERA
- Run pyMAMBA
- Update calibration parameters
- Evaluation of error
- Apply detector surrogate

VERA Output Files
MPACT Surrogate

• Goal: Provide a (fairly) accurate detector response as a function of MAMBA parameters
• Looks at detector deviation compared to VERA run without crud/boron mass
  – Feeds in total core boron mass, assembly boron mass, axial boron mass, assembly power, assembly exposure
  – Uses Gradient Boosting Regression to fit the data
• Use “hand calibration” runs from FY18 milestone to train surrogate
  – Train with 75% of the data (6 runs, 20 statepoints, 56 assemblies), validate with 25%
Current MPACT Surrogate

Flattened Index of run, state, assembly, and axial level

Deviation in detector signal

Variable Importance

- Core Bmass
- Core Bmass * Axial Index
- Axial Index
- 2D Asy Power
- Neigh 2D Asy Power
- Axial Bmass
- 2D Asy Power * Axial Index
- Axial Bmass * Axial Index
- Neigh 2D Asy Power * Axial Index
- Neigh 2D Asy Bmass * Axial Index
- 2D Asy Bmass * Axial Index
- 2D Asy Power * Axial Bmass
- Neigh 2D Asy Bmass
- 2D Asy Exp
- 2D Asy Bmass
- 3D Asy Bmass

Relative Importance
pyMAMBA Driver

• Provides python bindings for MAMBA
  – C-bindings / Cython / numpy / mpi4py / h5py
• Provides capability to drive multicycle crud calculations
  – Integrates source term with crud growth
  – Uses VERA output files as input for boundary conditions
  – Provides mechanism to shuffle/remove crud between cycles
• Recent high-level driver development:
  – Provide low-barrier-to-entry, performant, parallel crud growth capability
  – Interoperable with standard VERA H5 output
  – Central component in a larger multi-cycle, core scale mamba calibration effort
  – Can operate as a standalone crud scoping tool
Calibration Sequence

Run coupled VERA → VERA Output Files → Run pyMAMBA → Update surrogate → Update calibration parameters → Evaluation of error → Apply detector surrogate → Run coupled VERA

- Calibration Sequence
- Run coupled VERA
- VERA Output Files
- Run pyMAMBA
- Update surrogate
- Update calibration parameters
- Evaluation of error
- Apply detector surrogate
Watts Bar Cycles 6 and 7 Core Calibration (Preliminary)

3D Detector RMS vs Exposure [EFPD]

- Calibrated MAMBA
- No MAMBA

Cycle 6
Cycle 7
CRUD Layer two-phase model

Two-phase models correlations has been developed for two-phase flow within the CRUD layer. Model is based on HEM (homogeneous equilibrium model) approach.

<table>
<thead>
<tr>
<th>Conservation Equation</th>
<th>Unknowns</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass, $\frac{\partial [\rho(s)u_x]}{\partial x} = 0$</td>
<td>$u_x$ and $s$</td>
<td>$s = \text{liquid saturation (1 - void fraction)}$</td>
</tr>
<tr>
<td>Momentum, $u_x = -\frac{K}{\mu(s)} \frac{\partial p}{\partial x}$</td>
<td>$u_x$, $s$ and $p$</td>
<td></td>
</tr>
<tr>
<td>Liquid Mass, $\frac{\partial}{\partial x} [\rho u_x \lambda_1] = -\frac{\partial}{\partial x} \left( \frac{K}{v(s)} \lambda_1 \lambda_\nu \frac{\partial p_\nu}{\partial s} \frac{\partial s}{\partial x} \right) + \dot{m}_l$</td>
<td>$u_x$ and $s$</td>
<td>$\dot{m}<em>l = \frac{\dot{Q}}{h</em>{vl}}$</td>
</tr>
<tr>
<td>Energy, $(\rho c_\nu u_x) \frac{\partial T}{\partial x}$</td>
<td>$u_x$, $s$ and $T$</td>
<td>$Q = \text{heat transferred from the solid matrix to the two-phase mixture}$ $h_{vl} = \text{enthalpy of vaporization}$ Depends on the heat transfer regime within the CRUD layer. This will also appear as a sink term in the heat conduction equation of the solid CRUD</td>
</tr>
</tbody>
</table>

Huxford, A., Manera, A., NURETH 19
CRUD Layer two-phase model

- Change in slope of boiling curve for crudded rods due to changes in heat transfer regime (observed in WALTLOOP data)
- Validated correlations for HTC have been identified and will be implemented in two-phase CRUD model ($\dot{Q}$ term in Energy balance eq.)
  - Wick boiling
  - Departure from wick boiling (dryout)
  - Film boiling
Calibration of the reaction rates is currently underway using Callaway Cycle 9 crud scrape chemical analysis (work in progress)

- Callaway Cycle 9
  - Axial offset of -15%
  - Downrating of reactor power by 30%
  - Bonaccordite (Ni$_2$FeBO$_5$) made up >50% of certain crud samples
  - Thickest samples range 50-100µm

Radial profile of a crud sample compared to MAMBA's simulation at the end of cycle:

SEM micrograph of a CRUD scrape from the Callaway plant showing needle-shaped bonaccordite crystals

Radial Composition Profile of Callaway Cycle 9 crud predicted by MAMBA

- Both Ni metal and NiFe$_2$O$_4$ surface deposition occurs
  - NiFe$_2$O$_4$ deposition gives way to Ni deposition as the deposition rate increases, filtering NiFe$_2$O$_4$ from the coolant, leaving only Ni metal to deposit
- Ni and NiFe$_2$O$_4$ react with the soluble species inside the crud to form Ni$_2$FeBO$_5$
- Bonaccordite (Ni$_2$FeBO$_5$) and lithium tetraborate (Li$_2$B$_4$O$_7$) exist in high concentrations
  - => together they cause significant AOA
Questions?