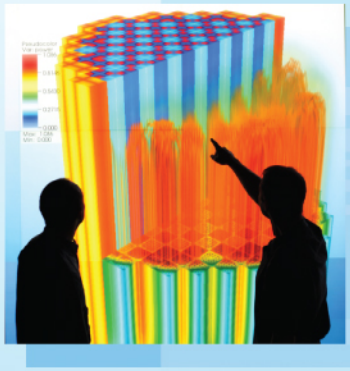
Power uprates
and plant life extension

CASL-U-2011-0175-000

Consortium for Advanced Simulation of LWRs



Engineering design
and analysis

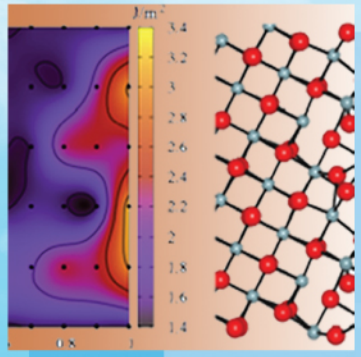
A 2D, High Resolution, Coupled Demonstration and Assessment of the Crud Challenge Problem

Brian Kendrick,
Los Alamos National Laboratory (LANL)

Michael Short
Massachusetts Institute of Technology
(MIT)

Science-enabling
high performance
computing

August 26, 2011



Fundamental science

Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

MPO.Y2.01: A 2D, high-resolution, coupled demonstration and assessment of the crud challenge problem

Brian Kendrick[1*] and Michael Short[2]

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[1]Los Alamos National Laboratory (LANL), Los Alamos, NM 87545

[2]Nuclear Science and Engineering Department, Massachusetts Institute of Technology (MIT), Cambridge, MA 02139

[*]Corresponding Author, Phone: (505) 667-0856, Email: bkendric@lanl.gov

This report is prepared as part of the CASL-MPO effort on the crud project. This report is a deliverable for the following milestones:

- L3 Milestone: Demonstrate coupled 2D crud simulation with boron hideout (L3, 8/15/11)
- L2 Milestone: "MPO.Y2.01 – Conduct a 2D, high-resolution, coupled demonstration and assessment of crud challenge problem" with VRI (8/26/11)

CASL-U-2011-0175-000

1. Introduction

The problem of corrosion product build-up on the upper spans of fuel rods in PWRs is one of the key problems limiting reactor performance, power up-rates, and fuel cycle extensions. These corrosion products, known as crud (Chalk River Unidentified Deposits), hamper reactor performance in two ways. First, their porous nature results in a low thermal conductivity, leading to hotter regions in the fuel cladding beneath. This can lead to accelerated corrosion, known as CILC (crud Induced Localized Corrosion). Second, the pores provide a large volume for boron-bearing compounds to "hide-out" and concentrate. Boron is naturally present in PWRs as boric acid, which is used to control reactivity. The buildup of boron and the precipitation of boron-bearing compounds in the crud can lead to an axial offset anomaly (AOA), also known as CIPS (crud Induced Power Shift). This occurs when boron builds up inside crud in the upper spans of the fuel assemblies, locally depressing the neutron flux. This condition can lead to mandatory plant derating and a decreased shutdown margin for the plant.

The MPO focus area of CASL is actively developing a code to understand and predict the evolution of crud throughout the fuel cycle. This code, called MAMBA (MPO Advanced Model for Boron Analysis), can predict crud growth and composition, boron hideout, and elevated temperature distributions due to crud buildup. MAMBA has been designed as a first-principles code, capable of understanding crud at the microscale as well as the engineering scales. The code uses atomistically-informed parameters (such as rate constants, activation energies, diffusion coefficients, and thermal conductivity) and crud agglomeration mechanisms as fixed inputs to its microscale and engineering scale modules to add scientific basis to otherwise empirical calculations. The microscale model provides detailed temperatures, fluid velocities, and B/Li-bearing species concentrations around a single boiling chimney as functions of time, location, inputs (such as cladding heat flux and neutron flux), and operating history. Relevant outputs from the microscale module are then averaged into the engineering scale module, which computes crud thickness (growth), baseline porosity and composition. Relevant outputs from the engineering scale module, such as crud thickness, average thermal conductivity, and average boron concentration are then passed to VRI for integration into other focus areas, such as neutronics, thermal-hydraulics, and computational fluid dynamics groups.

This report documents the initial development phase of MAMBA v1.0 at both the engineering and micro-scales and its initial application to the crud test problem: a single-rod autoclave experiment. The MAMBA v1.0 computer code represents the first realization of the crud materials modeling framework defined in a previous report.[1] This framework is briefly reviewed in Sect. 2.1. Preliminary high-resolution two-dimensional (2D) MAMBA simulation results for crud deposition along a single PWR fuel rod are presented in Sect. 2.2. Sections 3.1-3.2 discuss the micro-scale module for the 2D FEM boiling chimney and boron deposition models. Simulation results for the micro-scale module are presented in Sect. 3.3. The coupling of the micro-scale module to the engineering scale MAMBA module and the VRI is discussed in Sects. 3.4-3.5. Summary discussion and future work are discussed in the final Sect. 4.

2. Engineering Scale Module

2.1. The Crud Materials Modeling Framework

A schematic of the crud materials modeling framework is shown in Fig. 1. The MAMBA computer code will leverage off existing capabilities in BOA and ChemPaC and will couple the various micro-scale models which describe the deposition of crud. Separate atomistic calculations will support the development of the micro-scale models by providing the needed parameters, such as: rate coefficients, activation energies, diffusion coefficients, solubilities, and thermal conductivities.

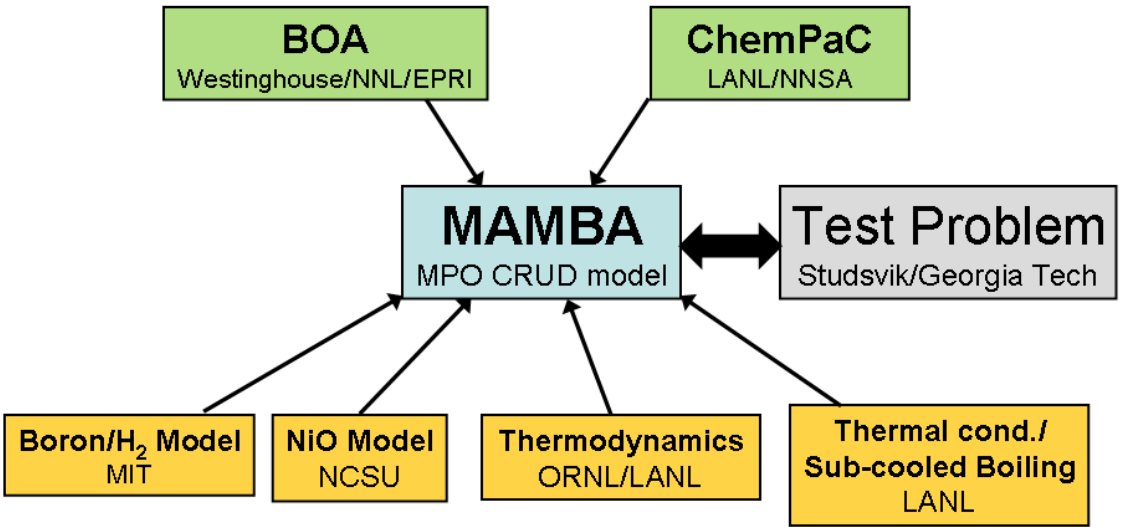

Figure 1: Crud materials modeling framework: MAMBA (MPO Advanced Model for Boron Analysis). MAMBA is a multi-scale coupled physics computer code describing the deposition of crud along the surface of a PWR fuel rod.

The macro or engineering scale module for MAMBA v1.0 is based on parts of ChemPac which have been modified to treat crud deposition along the surface of a single fuel rod. The initial version of MAMBA is two-dimensional (2D) with the computational grid consisting of grid points along both the axial direction of the fuel rod and the radial direction perpendicular to the fuel rod's surface (see Fig. 2). The primary inputs to MAMBA at the engineering scale include: (1) the heat fluxes or temperature profiles at the crud/cladding and crud/coolant interfaces, (2) the local heat fluxes within the crud due to sub-cooled nucleate boiling (SNB), and (3) the coolant concentrations of the various particulate and soluble species of interest. The primary outputs from MAMBA at the engineering scale include (all are functions of time): (1) the crud thickness, (2) the temperature distribution within the crud, and (3) the local concentrations of the various species of interest within the crud. From these MAMBA outputs the relevant risks for AOA and CILC can be assessed with much higher precision than was previously possible. In regards to AOA, the boron concentration will be computed as a

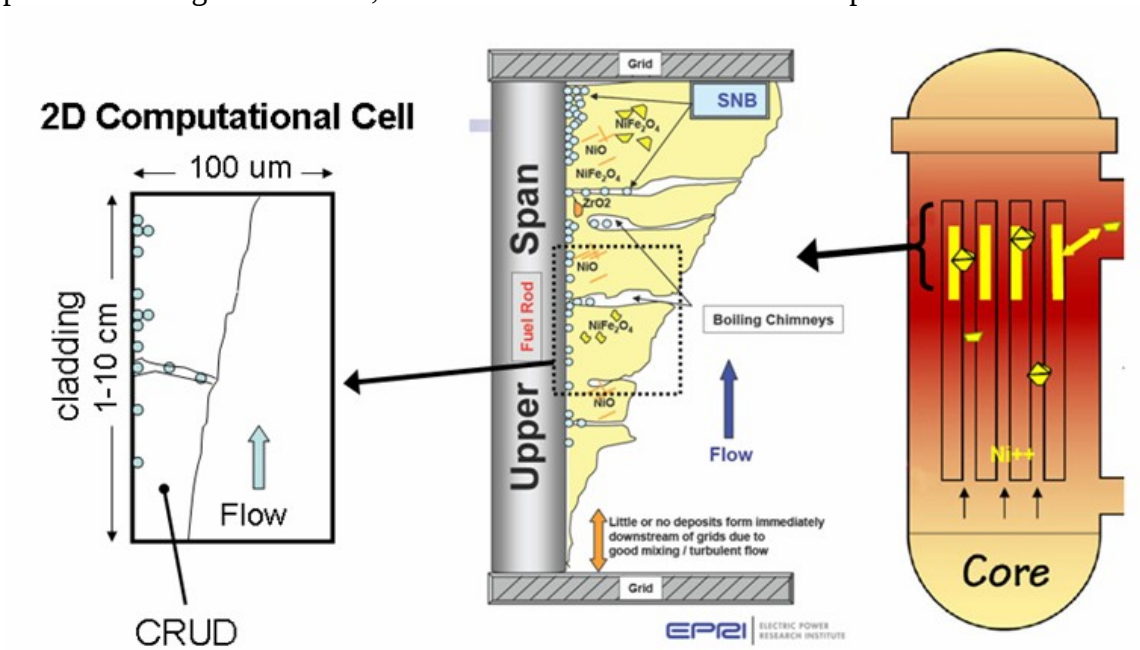

Figure 2: Schematic showing the MAMBA's 2D computational cell and how it relates to a single fuel rod in a PWR core.

function of time and precise location (i.e., <1 cm) on a single rod accounting for the local variations in the coolant flow and heat transfer in the core. In regards to CILC, the local temperature and concentration of lithium at the crud/cladding interface will be precisely determined.

The primary interface between the macro and micro-scale modules within MAMBA include: (1) the chemical kinetics equations describing deposition/precipitation at each computational node, and (2) the local heat flux leaving a control volume element due to SNB. Each of these interfaces contains at least two user-selectable models: (a) an empirical based model consisting of a reduced equation set with parameters determined either by fitting experimental data or from benchmarking against more fundamental models, and (b) a full set of kinetics equations and/or micro-scale model (see Fig. 3). For example, in regards to (1)-chemical kinetics, the current MAMBA empirical chemistry model is similar to that used by BOA and consists of a single first-order rate equation describing the overall surface deposition of $NiFe_2O_4$. The deposition rate is determined by fitting the crud thickness and mass to available plant data. Similarly, the empirical boron deposition is also described by a single first-order rate equation describing the precipitation of $Li_2B_4O_7$ (lithium tetraborate) within the crud. The deposition rates for both $NiFe_2O_4$ and boron include both boiling and non-boiling contributions.

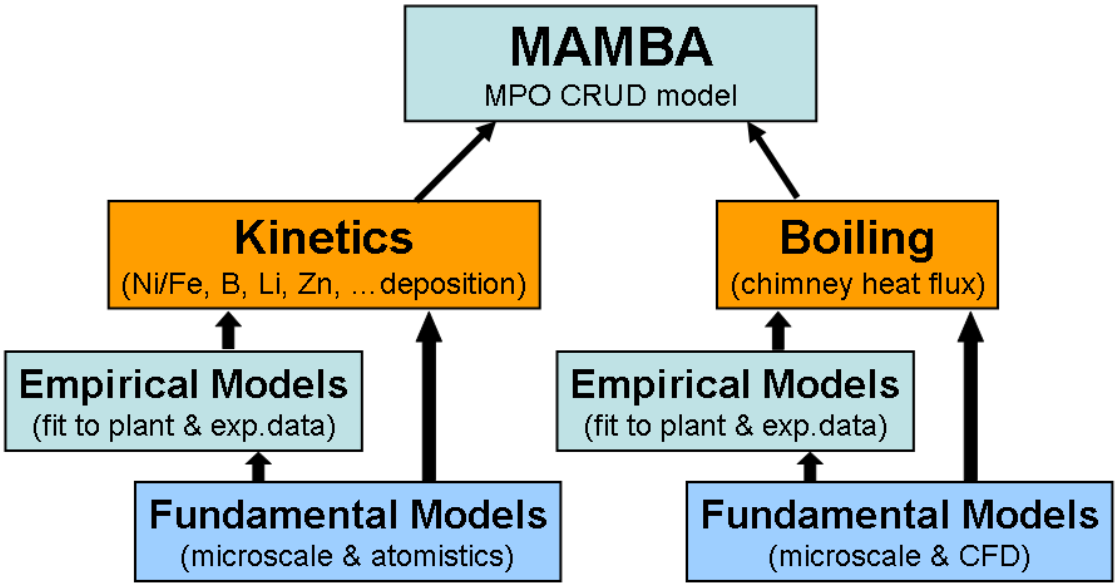

Figure 3: Schematic showing the relationship between MAMBA's empirical based models and the fundamental models for the deposition/precipitation kinetics and the local heat flux due to sub-cooled nucleate boiling.

The former are proportional to the local heat flux due to SNB. A detailed explanation of these models will be presented in a future report.[2] These simple empirical models are computationally fast but they do not contain the detailed chemical kinetics and transport associated with multi-species, catalytic surface deposition and precipitation reactions in porous crud. The fundamental kinetics and transport models are currently under development by the MPO-crud group and will be incorporated into MAMBA as they become available. The current fundamental micro-scale model for boron deposition is described in Sect. 3. In regards to (2)-local heat flux due to SNB, the current MAMBA empirical model is based on multiplying the total chimney surface area within a control volume element by a heat transfer coefficient, porosity, and the difference between the local crud temperature T and chimney fluid saturation temperature T_{sat}. In this model, the

effective SNB heat transfer coefficient and the average crud thermal conductivity were initially based on values used by BOA and then optimized by fitting the computed crud temperature distribution to experimental data (i.e., the WALT loop Ref.[3]). The current fundamental micro-scale model for computing the SNB heat flux is based on a 2D FEM boiling chimney model described in Sect. 3. The choice between using an empirical or micro-scale model is user selectable and the primary trade-off is computational efficiency for highly resolved kinetics and transport. The scale of the particular engineering application and available computing resources will often dictate which models to select. The empirical and micro-scale models can also be used simultaneously during a simulation. The selection of a particular model within a control volume can be automated based on the local conditions and previous benchmark studies. Alternatively, the micro-scale models can be called on a coarser grid (see Sect. 3.4 for an example).

2.2. MAMBA v1.0 Simulation Results

MAMBA v1.0 has been used to simulate 400 days of crud deposition along a single fuel rod (4m long by 2.54 cm in diameter) under PWR conditions. Results from the simulation are plotted in Figs. 4 and 5. Figure 4 plots the temperature distribution T(r,z,t) (colored contours) throughout the crud as a function of time.

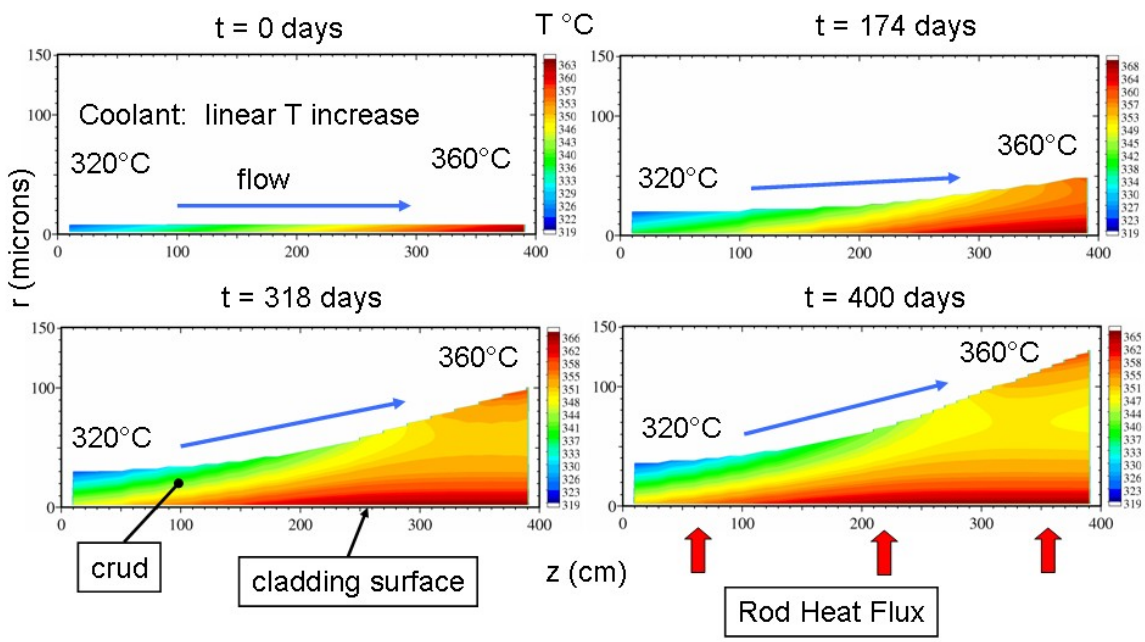

Figure 4: MAMBA v1.0 demonstration simulation of crud deposition along the surface of a single PWR fuel rod over a 400 day period. The colored contours are the temperature.

The surface of the crud grows continuously due to the deposition of Ni-Fe oxides on the surface. The growth rate is slower (faster) on the left (right) side of the plot due to non-boiling (boiling) conditions. The mass deposition at each point on the surface is calculated at each time step from a numerical solution of a first-order rate equation. A constant temperature profile at the coolant/crud interface is used which increases linearly from 320C on the left edge (z = 0) to 360C on the right edge (z = 4m). A constant and uniform heat flux of 1.26×10^6 W/m^2 is used at each point along the crud/cladding interface (r = 0). The computational grid consists of 40 points equally spaced by 10cm along z. An adaptive time-dependent grid is used in the radial (r) direction which automatically adds points as mass is deposited on the crud's surface. A grid spacing of 2 microns is used in r. The temperature distribution T(r,z,t) was computed using a standard finite-difference approach for solving the time-dependent (2D) heat transfer equation in r and z at each time t including a local SNB heat sink term. A variable time step is used which starts at 10usec at the beginning of the simulation and quickly increases to 100s as thermal equilibrium is reached. Depending upon the grid size, the entire 400 day simulation can be done in as little as 3.4 minutes of CPU time. Figure 5 plots the boron concentration as a function of time. The boron deposition model used in this particular simulation is an empirical model based on the numerical solution of a first-order rate equation.

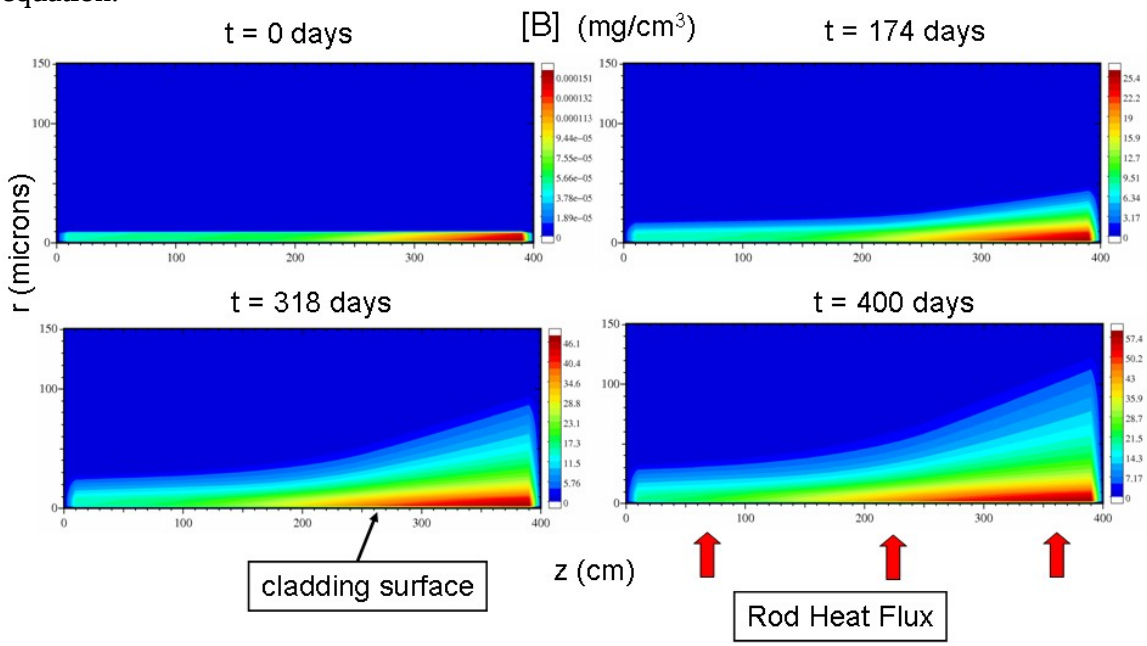

Figure 5: MAMBA v1.0 demonstration simulation of boron concentration (colored contours) inside the crud deposit (see Fig. 4) along the surface of a single PWR fuel rod over a 400 day period.

As expected, boron concentrates in the hottest regions with the most SNB. Future simulations will utilize the micro-scale boron deposition model discussed in Sect. 3. The details of the numerical techniques, the adaptive grid, deposition rate equations, and all of the parameters used in the calculation will be discussed in a future report.[2] Movie files for each of the simulations plotted in Figs. 4 and 5 are available upon request (they are in mpeg format and are about 5 MB in size).

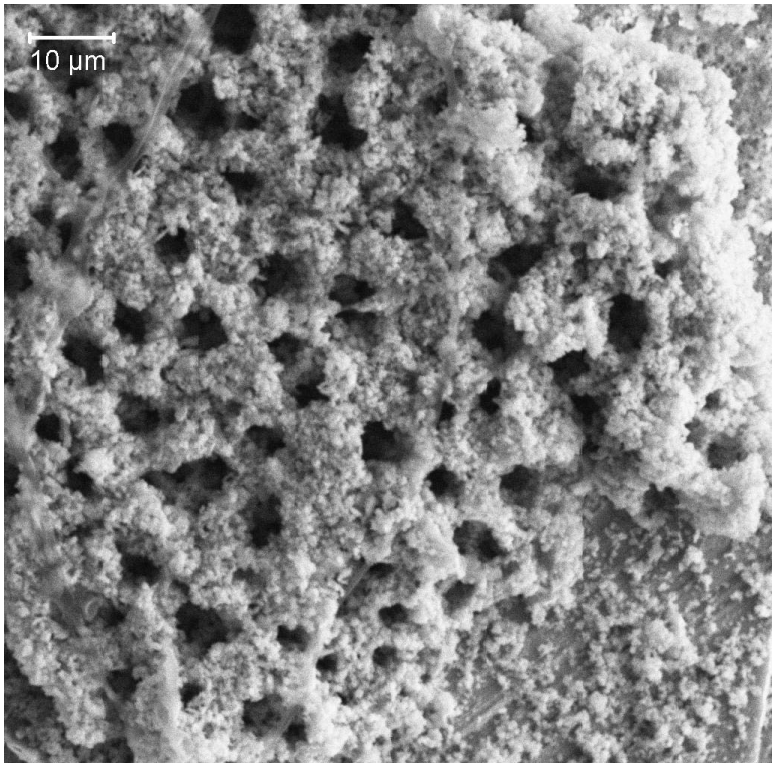

Figure 6: SEM image of crud scrape from a PWR fuel rod.[6]

The results of the simulations presented in Figs. 4 and 5 qualitatively reproduce the expected behavior of crud growth and boron deposition. Their primary purpose is to help more clearly define the crud modeling framework, the interfaces between the macro and micro-scale modules, and the external interfaces with the VRI. They demonstrate the goals and future research directions needed for the development of MAMBA but they are not yet a quantitative prediction of crud growth and boron deposition. Much work remains to fully develop and validate MAMBA. However, even in its present form MAMBA v1.0 can be used to begin the initial assessments and validation studies of the coupled physics and chemical kinetics models against the crud test problem: a single-rod autoclave experiment.[4,5] Sensitivity studies can also be used to explore which parameters are most important and need further development. Future improvements to MAMBA guided by experimental data and fundamental calculations will produce a fully validated coupled multi-scale model for simulating crud deposition at a quantitative level.

3. Microscale Module

3.1. Overall Description

MAMBA's microscale module focuses on solving the 2D temperature, fluid velocity, and species concentration profiles inside the crud around a single boiling chimney. Experimental observations of crud scrapes show the crud to be made of porous deposits with boiling chimneys, as shown in Figure 6.[6] Detailed SEM studies have shown the crud to be highly porous, allowing for fluid to wick into the crud from the coolant, evaporate at the chimney surface, and exit the crud as vapor.

The microscale model therefore focuses on the crud around one of these boiling chimneys.[7] A schematic of the control volume for the simulation, along with the processes occurring within, is shown in Figure 7. The crud for the simulation is assumed to be radially symmetric around the boiling chimney. Therefore, only a 2D slice of the

crud needs to be modeled. The code solves Laplace equations for temperature and fluid velocity distributions. It then assumes that during steady-state, the advection of boric acid due to coolant wicking balances out diffusional transport, which works in the opposite direction of fluid advection. The code also accounts for chemical reactions between boron- and lithium-bearing species, such as lithium tetraborate. Finally, isotopic fractions are tracked by the code as boron-10 is selectively burned, due to its far higher cross section for neutron capture. Each atom of boron burned then creates an atom of lithium, which is explicitly tracked by the code.

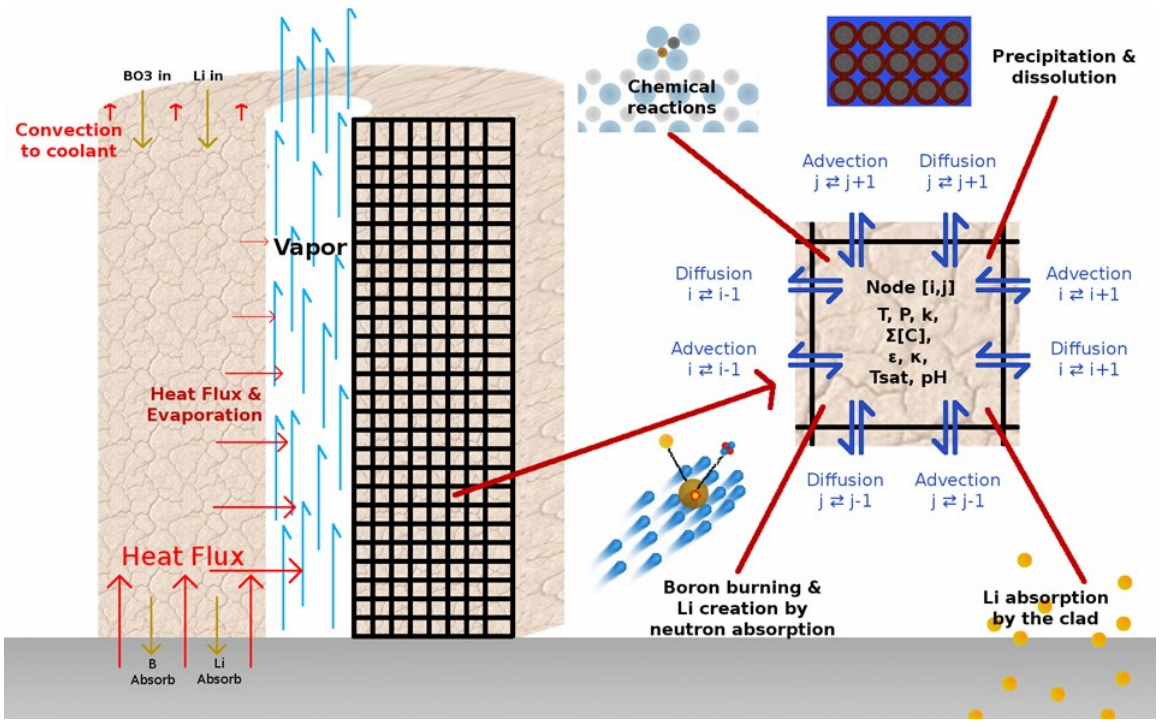

Figure 7: Schematic of crud geometry simulated by MAMBA's microscale module, with diagrams of processes modeled within.

3.2. Block Diagram

MAMBA solves for the three distributions mentioned above in an iterative fashion. A block diagram of the microscale module's code is given in Figure 8. First, the code collects its inputs. These come from a combination of parameters passed down by the engineering scale module (crud thickness, composition, skeletal porosity), from restart files (if previous simulations have taken place), from user inputs (for changing reactor conditions, such as cladding heat flux and neutron flux), and from default values for those not explicitly specified. The code then solves for the temperature distribution inside the crud. It assumes that the temperature of the fluid at the boiling chimney is pinned at the saturation temperature for the given concentration of boric acid in water. With this temperature distribution, the fluid velocity is found assuming that the heat flux at the chimney (found using dT/dx at the chimney) determines the mass flow rate, and therefore the fluid velocity. Finally, the concentrations of various chemical species, such as boric

acid and lithium ions, are found using the advection=diffusion assumption and the fluid velocity profile just found. This cycle is repeated until convergence is achieved.

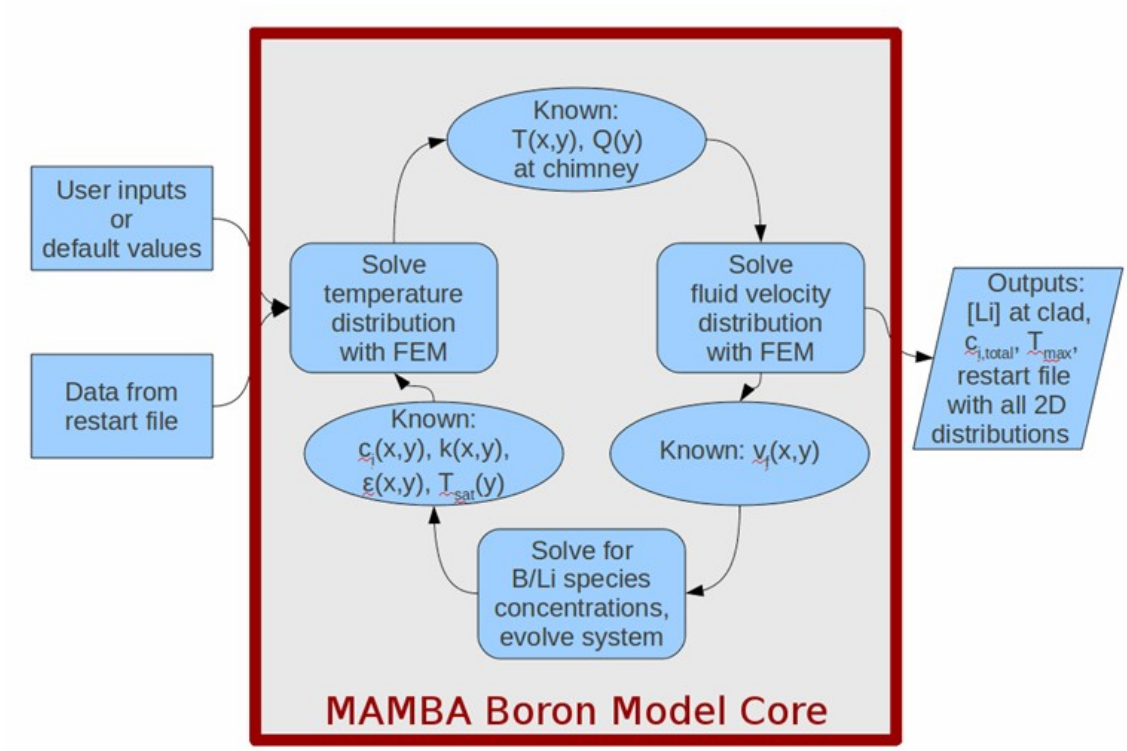

Figure 8: Block diagram of MAMBA's microscale simulation, showing the iterative process of arriving at 2D distributions.

3.3. Preliminary Results

An example of some preliminary results of MAMBA's microscale simulator is shown in Figure 9. In this figure, the temperature, fluid velocity, and boric acid concentration profiles have been solved for using the coupled physics described in Sections 3.1 and 3.2. The location of maximum temperature is on the fuel cladding, as far away from the boiling chimney as possible. The locations of maximum fluid velocity and maximum boric acid concentration are coincidental, on the cladding/crud/chimney interface. This is also the location of the highest evaporative heat flux. These coupled 2D simulations allow pinpointing of the locations and magnitudes of the highest temperatures and species concentrations. They are therefore the best indicator for CILC risk in VRI, especially when coupled with the appropriate zirconium oxide corrosion models from the PCI/Corrosion group in MPO.

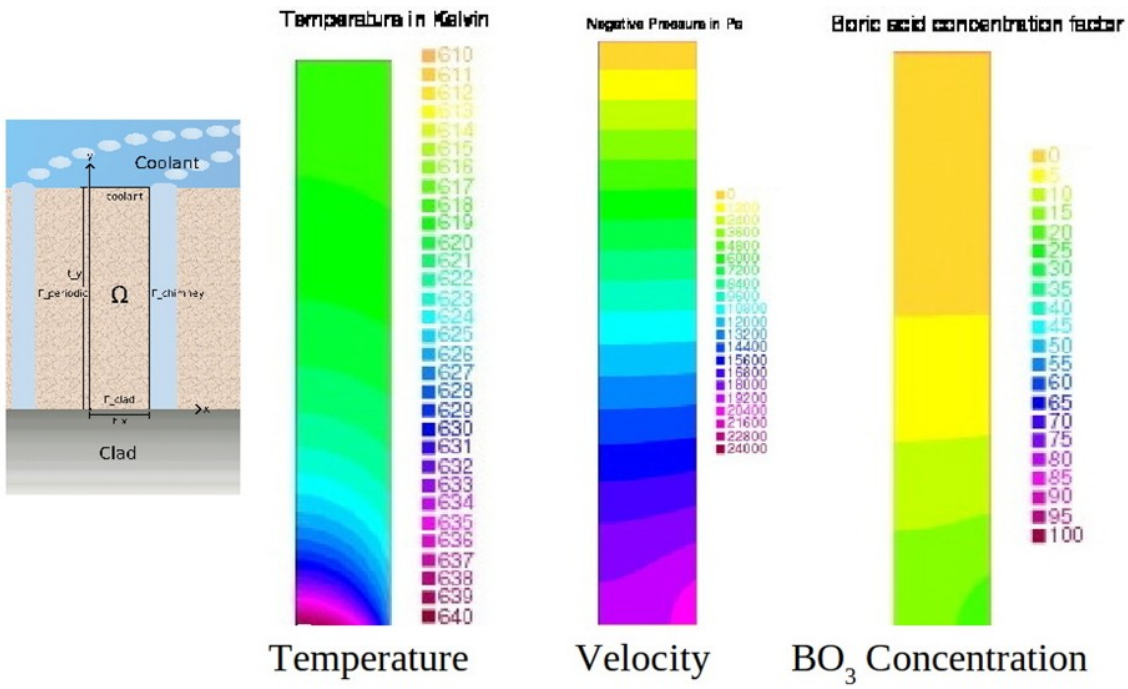

Figure 9: Preliminary results of MAMBA's microscale model using coupled physics. The crud geometry simulated is shown on the left for reference.

3.4. Direct Coupling to MAMBA Engineering Scale Module

MAMBA's microscale module is designed to off-load detailed calculations from the engineering scale module. It is intended to be called by the engineering scale module as a sub-routine, informing it with highly precise ultra-fine mesh calculations of temperature and species concentrations. The microscale module will be called at multiple locations along any given fuel rod, as shown in Figure 10. The averaged outputs of these microscale simulations will then be collected and interpolated by the engineering scale module. The number and frequency of these microscale calculations will be kept to a minimum, in order to decrease the amount of CPU-intensive calculations required to run MAMBA.

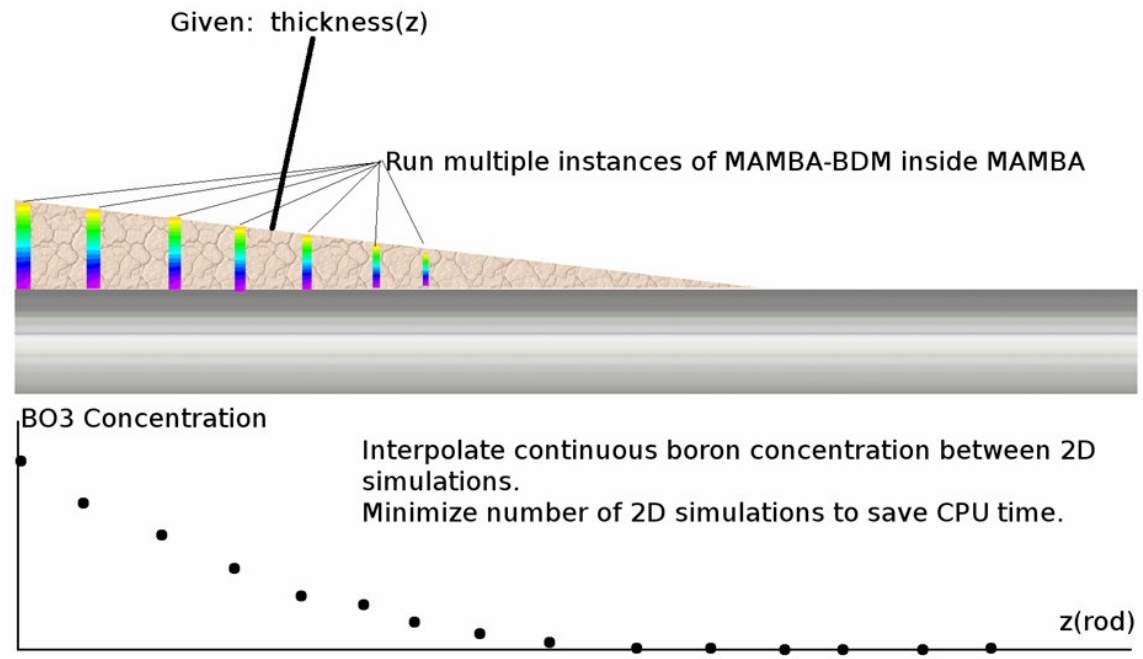

Figure 10: Schematic showing how MAMBA's engineering scale module calls the microscale module. This offloads many CPU-intensive calculations, allowing for interpolation between microscale simulations with minimal loss in accuracy.

3.5. Physical Coupling Mechanisms

MAMBA has been designed as a coupled-physics framework from the start. The methods by which physical models are coupled will be explicitly described in this section. First, temperature dependencies of all possible parameters, such as fluid viscosity, diffusion constants (themselves functions of viscosity) and thermal conductivities are modeled. The boric acid (and polyborate ion) concentration dependence of the saturation temperature of water is also taken into account. Next, the derivative of the temperature distribution determines the fluid flow at the crud/chimney boundary, which is one key boundary condition. This fluid velocity also determines the B/Li-bearing species advection velocities inside the crud, which are balanced out by previously mentioned temperature-dependent diffusion velocities. Concentration dependence of diffusion constants is not yet modeled, but is planned. Finally, aspects of the microscale model couple directly with other CASL focus areas. For example, the thermal hydraulics group updates MAMBA with accurate coolant temperatures, coolant pressures, and cladding wall heat fluxes. The isotopic concentrations of boron are also coupled directly to the neutronics calculations, and the boron concentrations are fed back to the neutronics group to iteratively find local neutron flux depressions, leading to a measurement of AOA.

4. Summary / Conclusion

The MPO crud materials modeling framework was reviewed. The initial implementation of this framework was described through the development of MAMBA (v1.0). MAMBA is a multi-scale coupled physics computer code describing the deposition of crud along the surface of a PWR fuel rod. The two primary modules in MAMBA were described: the engineering scale module and the micro-scale module. These modules are coupled within MAMBA. The engineering scale module represents the primary interface with the VRI and passes the external inputs and outputs to the micro-scale module. The micro-scale module is based on fundamental chemical kinetics and physics models. These fundamental (atomistically informed) models are currently under development by the MPO crud group and will incorporated into MAMBA as they become available. A preliminary 2D FEM based micro-scale model for the boron deposition within a single boiling chimney was described. MAMBA v1.0 was used to perform a 2D high-resolution demonstration calculation of the crud test problem: crud deposition along the surface of a single fuel rod. The results of this simulation include: the time evolution of the crud's thickness, the crud's internal temperature distribution, local heat fluxes within the crud due to SNB, and the boron distribution within the crud. The results from this preliminary simulation reproduce the expected qualitative behavior associated with crud deposition. However, much work is needed to develop a fully validated model which gives quantitative results for crud deposition under a variety of PWR conditions. The engineering and micro-scale modules in MAMBA will continue to improve and a full three-dimensional (3D) simulation capability will also be implemented in the future. The integration of MAMBA v1.0 with the other MPO groups (PCI and GTRF) and the rest of the VRI will also be implemented as these interfaces develop. This report fulfils the CASL MPO L2 milestone: "MPO.Y2.01 – Conduct a 2D, high-resolution, coupled demonstration and assessment of crud challenge problem".

5. References

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