CASL TechNotes

Consortium for Advanced Simulation of Light Water Reactors

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About Tech Notes

*CASL **Tech Notes** are produced by CASL's technical staff to spotlight areas of particular technical interest and to discuss CASL science and engineering innovation, accomplishments, activities, and plans. **Tech Notes** will be produced on a quarterly basis.*

In this Issue...

- Progress in THM Development
- CASL's Core Simulator and it's role in VERA
- CASL's Foray on CRUD

Progress in THM Development

The flow distribution within a Pressurized Water Reactor has a global influence on the generating efficiency of the unit. The circulating fluid is multifunctional; that is, it moderates the neutrons that fission to produce the reactor's power, it provides cooling to the fuel, and it also supplies the power plant's steam generators with the heat necessary to create electricity. Thus, the accurate prediction of the coolant flow and temperature (an application frequently termed "thermal-hydraulics" or "T-H") is essential to the accurate prediction of the reactor power and fuel integrity, and the local properties of the coolant has first order feedback effects on other local physical phenomena.

T-H analyses have historically relied on simplified computational approaches (e.g., channel flow models) established in the 1960s and 1970s. However, over the last two decades, significant advances in computing power have facilitated impressive advances in the field of computational fluid dynamics (CFD). Application of CFD to T-H analyses in Light Water Reactors, while in its formative stages, is providing new insights to coolant phenomena and serves as the foundation for an overall predictive simulation capability.

CASL's Thermal Hydraulics Methods (THM) team is focused on the development of a robust, accurate, and heavily tested (verified and validated) 3D CFD simulation capability for the VERA toolkit of applications. CASL's non-proprietary CFD application, Hydra-TH, uses a hybrid finite-volume/finite-element multi-physics approach for modeling single- and multi-phase flows with interphase mass and heat transfer. The development effort is intended to complement the capabilities in existing commercial CFD codes, such as CD-Adapco's STAR-CCM+ . **(p. 4)**

CASL's Core Simulator and its Role in VERA

The CASL vision is to confidently predict the performance of commercial nuclear power reactors through comprehensive, science-based modeling and simulation technology. To achieve this vision, CASL is assembling, assessing and coupling a variety of physics codes, each with a distinct purpose and functionality. This higher-fidelity coupled physics code capability is intended to have broad, versatile functionality with multiple modules simulating issues such as grid-to-rod-fretting and CRUD deposition; however, at the core of all reactor problems resides the primary physics required to derive the most basic information about the reactor's performance: neutron density; coolant temperature, flow rate and density; fuel temperature, isotopic composition, and clad integrity.

As the CASL Hub was established, it was recognized that the generalized codes earmarked for CASL didn't necessarily have support for modeling the very specific environment of a commercial power reactor - that is, the codes were not "reactor aware." For example, the neutronics codes did not include modeling options to simulate movable control rods or to shuffle fuel through multiple cycles, all standard requirements for industry applications. In order to ensure the necessary capabilities were incorporated into the codes, CASL instituted a development plan known as the "Core Physics **(p.2)**

CASL's Foray on CRUD

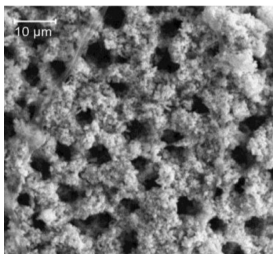

Fig. 1. SEM image of a PWR CRUD Flake (courtesy EPRI)

As the coolant in light water reactors is circulated through the primary loop, it carries along both soluble and particulate CRUD – nickel and iron corrosion products released by the steel and Inconel piping and components. CRUD deposits (an example is shown in Fig. 1) are typically porous, and sub-cooled boiling within the porous CRUD layer results in concentration of boric acid and lithium hydroxide within the CRUD. The porosity of CRUD can vary from deposit to deposit. Also, the porosity can vary through the thickness of the deposit, with lower porosity near the clad than on the waterside of the deposit.

In PWRs, thick CRUD deposits (25-50 microns) can result in boron compounds precipitating in the CRUD, affecting the local power production and inducing CRUD induced power shifts (CIPS). During core power maneuvers as coolant temperatures are reduced, the boron dissolves back into the coolant. The redistribution of the boron also alters the core. CIPS degrades shutdown margin, since the dissolution of boron after plant trip increases core reactivity. As operating PWRs have implemented power uprates and optimized fuel management strategies to improve fuel efficiency, **(p. 2)**

Coming in our next issue of ***TechNotes***:
VERA Status at a Glance . . .

CASL's Core Simulator and it's Role in VERA (continued from p. 1)

Benchmark Progression Problems" (listed in Fig. 2). This set of Progression Problems map out the step-wise implementation of capabilities necessary to create the identified "reactor-aware" environment and have been tagged by the team as the CASL "Core Simulator." The Core Simulator, or VERA-CS, capabilities correspond to an industry core cycle design simulator, although at much higher levels of fidelity and granularity. VERA-CS is a subset of the full intended CASL code capability and is further a subset of the primary physics required to derive the basic reactor core performance information. Once VERA-CS's development, led by VRI's Scott Palmtag, is complete per Progression Problem specifications (currently targeted for end of FY13), the "reactor-aware" capability will be an integral part of VERA, and the "-CS" moniker will be retired.

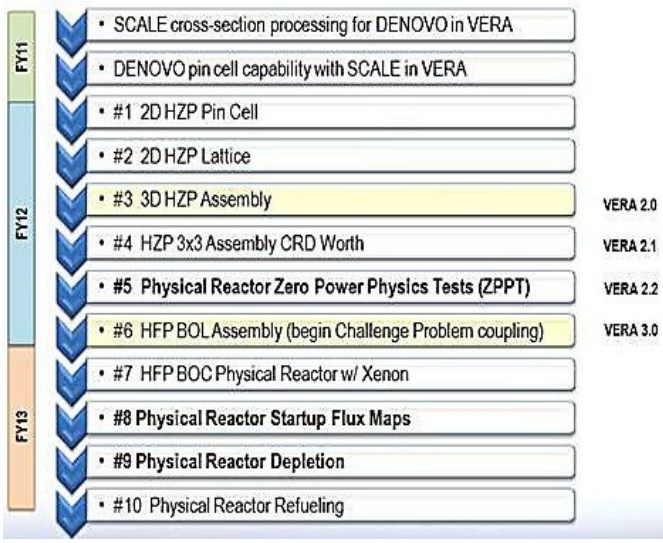

Fig. 2. AMA Core Physics Progression Problems

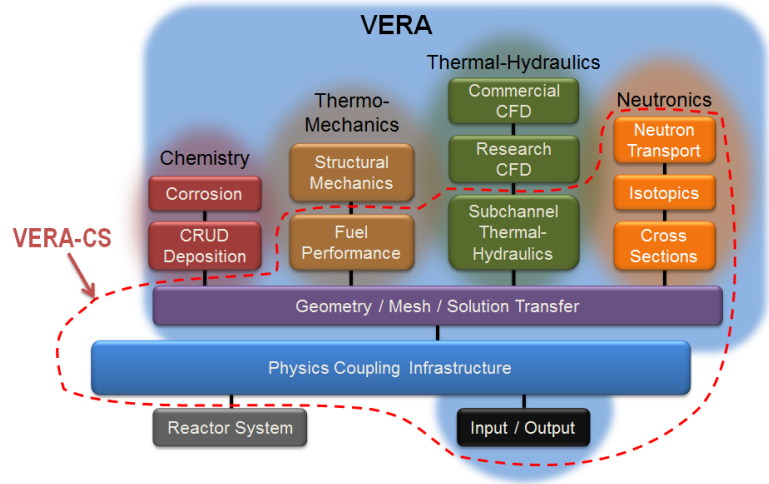

Fig. 3. VERA components that comprise VERA-CS

The implementation of the Core Physics Progression Problems has been very successful in driving the development of code capabilities within CASL, and the approach has been further adopted by Advanced Modeling Applications (AMA) to stimulate development in thermal-hydraulics and fuel rod performance. A rough outline of the T-H and fuel rod performance progression problems has been drafted by AMA Deputy Lead Steve Hess, and these are expected to be further refined early in CY2013.

The development of the Core Simulator has also spawned some supporting development such as the "VERA/Input." This summary input provides a systematic, human-readable, central input to the majority of the VERA codes. More information on VERA-CS is available at CASL-I-2012-0045-000.

CASL's Foray on CRUD (continued from p. 1)

CRUD deposition on fuel assemblies has become more prevalent. Higher heat fluxes associated with the power uprates leads to increased sub-cooled boiling rates in the core. As CRUD deposits thicken and densify, the deposits can impede heat transfer resulting in increased fuel cladding temperatures. Deposits that impede heat transfer can result in accelerated cladding corrosion and CRUD-induced localized corrosion (CILC). Fuel cladding leaks related to CRUD deposits have occurred in at least five pressurized water reactors (PWRs).

In order to predict and mitigate these effects, the commercial nuclear industry has developed several simulation methods and associated codes. Initial industry modeling focused on predicting sub-cooled boiling rates. In the late 1990's, work began to develop an integrated model that included CRUD and boron deposition within the CRUD. This model included an overall CRUD mass balance to determine the coolant corrosion product concentration, clean surface sub-cooled boiling models, CRUD deposition models, additional models for sub-cooled boiling on a crudded surface, and models for determining the concentration and precipitation of boron and lithium within the CRUD layer (Westinghouse BOB code, 1998 and subsequent EPRI BOA code, 2001). These codes generally predicted average and maximum CRUD thickness for the fuel assembly. In the late 2000's, the models were extended to predict local CRUD deposits on individual fuel rods as well as dryout within the local deposits. These models have led to a better understanding of the interaction between the various processes leading to CRUD deposition and fewer plants are now experiencing thick CRUD deposits leading to CIPS or CILC.

While current industry CRUD deposition tools have proven successful in reducing the occurrences of CIPS and CILC, much uncertainty remains about CRUD modeling. Improved models are needed in many areas, including the effect of coolant chemistry (in particular pH), operational transients such as plant trips or power maneuvers on corrosion source term release rates, feedback to local fuel rod heat flux from CRUD and boron deposition, sub-cooled boiling rates and CRUD chimney modeling, and boron concentration models. CASL is working to advance the state of the art in many of these areas; CRUD Product Integrator Jeff Secker (Westinghouse) is applying particular emphasis to the development of refined microscale CRUD deposition models that are coupled with higher fidelity local subcooled boiling predictions to capture the feedback between the insulating CRUD layer, the local coolant temperature and density, and the neutron flux and power. (p.3)

CASL's Foray on CRUD (continued from p. 2)

Physics Feedback and Necessary Coupled Solutions

Local flow rates and turbulence vary around the surface of individual fuel rods, and in the upper elevations of the core where there are high heat flux, local cladding surface temperatures, and bulk coolant temperatures, sub-cooled boiling can occur. The sub-cooled boiling can, in turn, result in CRUD precipitation and deposition on the surface of the rod. The CRUD deposits increase the clad surface temperature, increasing the potential for sub-cooled boiling and CRUD precipitation. However, in areas of high relative flow, the cladding temperature is reduced and local turbulence helps erode any CRUD that is deposited on the rod. The result is that CRUD is not uniformly deposited around the fuel rod surface and substantial azimuthal variation occurs, resulting in the striping often observed visually during inspections of fuel with CRUD deposits. Thus, there is a strong positive feedback between the local flow conditions, the local clad surface temperature, and the thickness of the CRUD deposited. Conversely, boron deposition within the CRUD deposits can provide a negative feedback mechanism. The deposition of neutron-absorbing materials (e.g., boron) captured within the CRUD reduce the local power. This reduces the local cladding temperature and sub-cooled boiling rate, eliminating or reducing further CRUD deposition.

Accurate local modeling of CRUD deposition therefore requires the use of coupled high-fidelity multiphysics including CFD (RANS) T-H representation, a neutron transport code capable of pin-resolved power predictions, and detailed CRUD and chemistry models. In an early step in demonstrating high fidelity CRUD predictions, CASL developed a preliminary CRUD modeling capability by coupling MAMBA, STAR-CCM+, and DeCART through a sequence of three separate coupling interfaces.

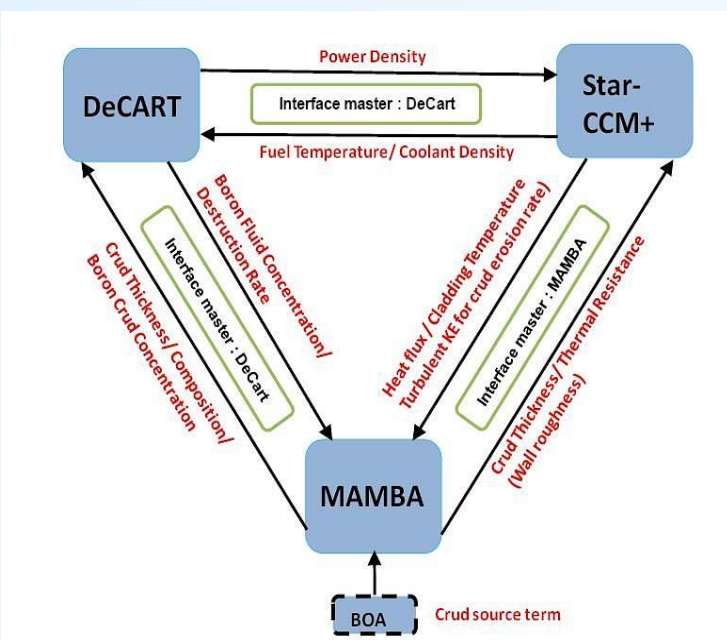

Fig. 4. Coupling components and data exchange used in the demonstration

CASL Crud Modeling with DeCART/STAR-CCM+/ MAMBA

MAMBA is a CASL-developed Fortran-based computer code that simulates three-dimensional crud growth along the surface of a fuel rod. Brian Kendrick (LANL) and University of Michigan researchers Dr. Annalisa Manera, Dr. Victor Petrov and PhD candidate Dan Walter completed a demonstration last year that illustrated the necessary physics coupling, utilizing manually exchanged and iterated solutions from the three individual two-way coupled physics pairs, as illustrated in Figure 4. In the future, the calculations will be automated under LIME, CASL's physics coupling environment.

For the demonstration, the first step was executing the coupled neutronics/thermal-hydraulics solution. The DeCART code provided STAR-CCM+ with the volumetric heat rate in the fuel pin for each CFD mesh, while STAR-CCM+ supplied DeCART with fuel temperature and fluid density distributions for each neutronics mesh. Next, the coupled thermal-hydraulics/CRUD deposition solution was executed, given the inputs supplied by the first step in the process. MAMBA provided the additional thermal resistance between the cladding and fluid introduced by the CRUD formation on the cladding surface. The CRUD thermal resistance is a function of the thickness, porosity and thermal conductivity of the CRUD layer. The accumulation of a CRUD layer on the cladding surface also has an influence on the wall roughness; however, this effect was not taken into account in the demonstration. Future studies will be performed to analyze its importance on the thermal-hydraulic predictions.

STAR-CCM+ provided the heat flux, the cladding temperature and the fluid temperature distributions needed to calculate the CRUD growth. The turbulent kinetic energy in the proximity of the cladding surface needed for the estimation of the CRUD erosion was also provided by STAR.

Finally, the local boron concentration and CRUD thickness were calculated by MAMBA and passed to DeCART. In the current MAMBA code set both the $NiFe_2O_4$ concentration and boron concentrations are calculated. Other relevant species will be added in the future. No information was passed from DeCART to MAMBA as a part of the demonstration; however, a data exchange for the computed boron depletion has now been implemented.

For this demonstration, the coolant chemistry was supplied by an ex-core model (e.g. BOA) and consisted of the standard inputs: boron concentration (ppm), lithium concentration (ppm), H_2 concentration (cc/Kg), soluble Ni (ppb), soluble Fe (ppb), and particulate $NiFe_2O_4$ concentration (ppb). The various CRUD properties used by MAMBA are currently based on CRUD measurements taken from operating PWRs and Westinghouse WALT loop studies (EPRI, 2011) and include porosity, CRUD density, CRUD thermal conductivity, average chimney radius, and average chimney density. The bulk properties of the CRUD (such as its thermal conductivity) are computed using a standard "mixing fraction": $k = (1 - \varepsilon)\, ks + \varepsilon\, kw$, where ks is the thermal conductivity of the solid CRUD ($NiFe_2O_4$) and kw is the temperature dependent thermal conductivity of the water filling the pores of the CRUD and ε is the time-dependent local porosity. (p.5)

Progress in THM Development

(from p. 1)

In fiscal year 2012 (FY2012), several studies were completed to demonstrate CASL's initial T-H capabilities. One essential study was aimed at producing a minimal set of test and benchmark cases that CASL can exercise to gain confidence that the underlying physical models and numerical methods have the necessary fidelity.

The benchmark cases must possess the inherent geometric and physics complexities of the CASL Challenge Problems (such as GTRF, CIPS, and DNB) while also taking advantage of the available validation data. The initial list of cases developed runs the gamut from natural convection to two-phase forced flow and is intended to encompass the THM VERA requirements, although THM Focus Area Lead Mark Christon expects the benchmark list to expand in the future.

A University of Michigan-based research team (I.M. Asher, T.J. Drzewiecki, T.P. Grunloh, V.E. Petrov, K.J. Fidkowski and A. Manera) has also completed a sensitivity, verification and validation study of STAR-CD, STAR-CCM+ and Nphase boiling models. CASL is currently using STAR-CCM+ in several single-phase simulations, and an ongoing Pilot Project led by Westinghouse engineer Jin Yan will utilize STAR's boiling models. Star-CD employs an Eulerian multiphase model that is representative of the treatments in other commercial codes. Boiling is modeled by a variation of the Kurul-Podowski heat-partitioning model. Star-CD served as the baseline reference code for the study, and provided heat-partitioning data to Nphase. Nphase was developed at RPI, and this finite volume parallel code can handle 2- and 3-D unstructured grids and includes multiple multiphase models.

This study yielded many findings, one being that the Kural and Podowski bubble size formulations typically overestimate the cross-section averaged void fraction in low void fraction ranges and underestimate it in higher void fraction ranges (Fig. 5). In the low void fraction range, improved predictions result when the more sophisticated S-gamma bubble size model is employed; however, this model does not yield improved results in the higher void fraction range. Further research of the bubble coalescence and break-up terms are therefore needed to improve the model's predictability (Fig. 6). The study also highlights the need to consider the effect of local fluid temperature on the liquid's thermodynamic properties.

In FY2013, CASL's T-H team will push to complete and demonstrate the supporting infrastructure in Hydra-TH for modeling single- and multiphase flows. Hydra-TH uses semi- and fully-implicit pressure-based projection algorithms for flow problems at low or moderate Mach numbers and is designed to incorporate both well established and state-of-the-art turbulence models, ranging from Reynolds-averaged Navier-Stokes (RANS) models to large eddy simulation (LES) techniques to various hybrid RANS-LES models. RANS models include the Spalart-Allmaras model and various flavors of turbulent-viscosity models (e.g. k-ϱ, k-ω). Available LES and hybrid RANS-LES variants include the monotonically integrated (or implicit) LES model, and different explicit treatments for the unresolved scales, e.g. the Smagorinsky, wall-adapted LES (WALE), the variational multi-scale, and detached-eddy simulation (DES) models. For multiphase flow problems, Hydra-TH solves ensemble-averaged governing equations for phasic conservation laws and a single pressure. Current focus is on implementation and verification of the N-fluid solver for multi-phase flow, (p.5)

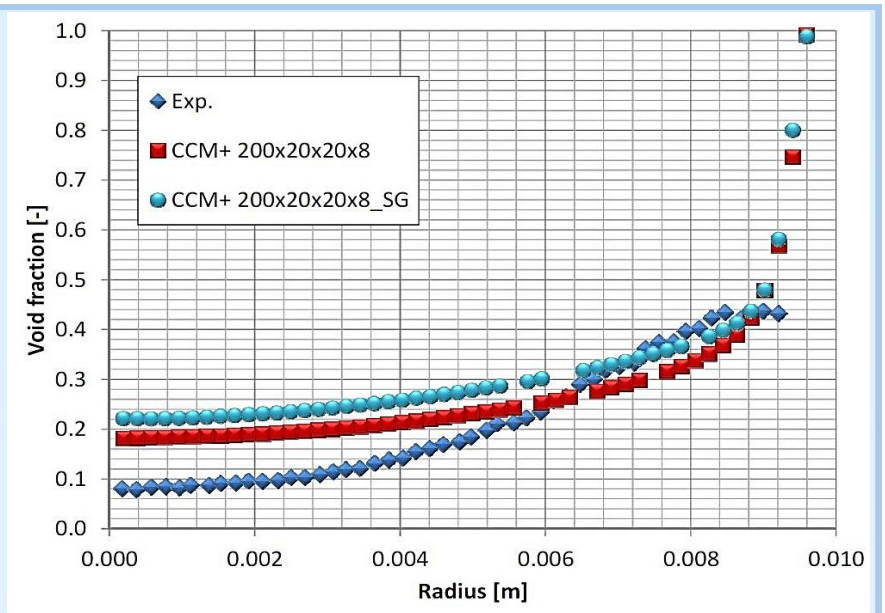

Fig. 5. A comparison of the CFD simulation results with experimental data

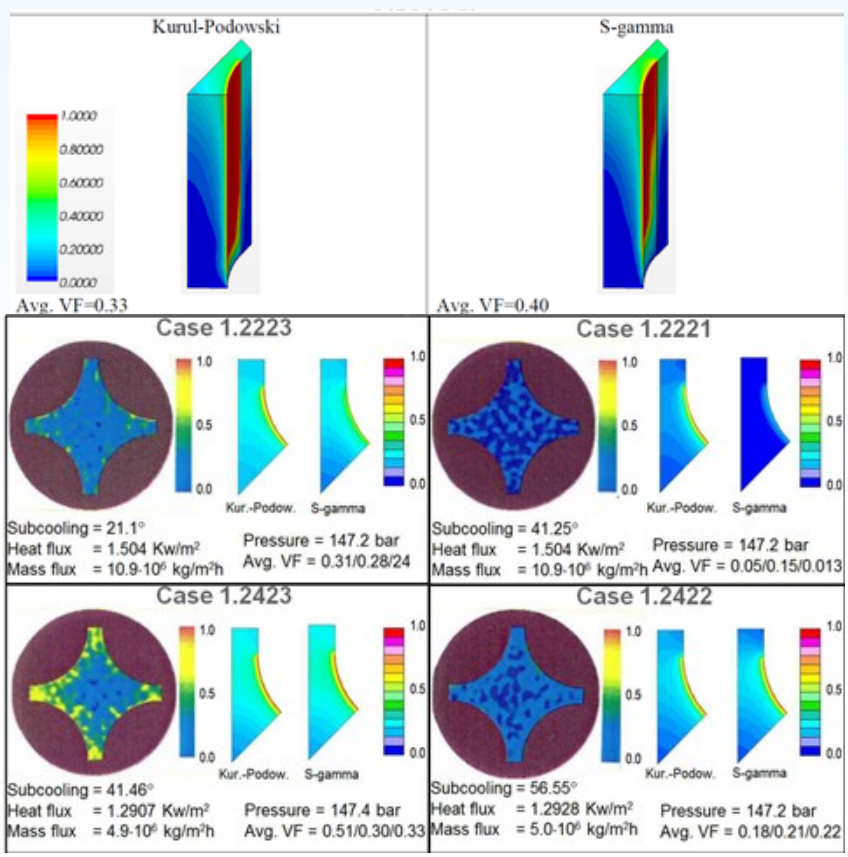

Fig. 6. Comparison between K-P and S-gamma bubble size models

CASL's Foray on CRUD (continued from p. 3)

Microscale calculations are being used to provide thermodynamic data that are input to MAMBA to broaden CRUD compositions predicted. Figure 7 provides an illustration of the calculation steps and results for this demonstration simulation. More information on CASL's CRUD deposition modeling strategy and the methods implemented within CASL's MAMBA code are available at CASL-I-2012-0045-000.

For CIPS and CILC modeling using advanced CASL codes, a two-tiered approach will be pursued. For CIPS, full core modeling is necessary to accurately determine the distribution of crud throughout the core. Early CASL experience suggests that pin-resolved transport linked to CFD, crud, and fuel performance models will be too computationally intensive, even on large super-computer clusters, to be practical, so sub-channel T-H methods will likely need to be used. These can be augmented with stand-alone CFD models to capture the axial and azimuthal variations in heat transfer components for each fuel rod. The expected data flow for this process is shown in Figure 8.

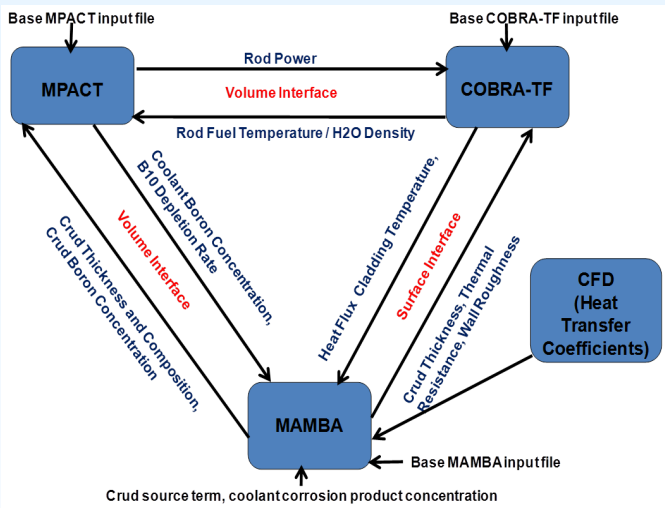

Fig. 8. Expected CRUD simulation data flow using CASL advanced codes

Progress in THM Development (from p. 4)

with initial calculations focusing on demonstrating turbulence single-phase and laminar multi-phase flow capabilities. These studies will be followed by further multi-phase flow modeling efforts that incorporate sophisticated solution algorithms and advanced closure models. Additionally, the THM team plans to integrate a library for generating and interpolating steam tables for multi-phase flow solvers. This will provide highly accurate equation of state evaluations, along with being fast for use in multi-phase CFD codes.

It should also be noted that CASL will offer a channel flow modeling capability, COBRA-TF, within VERA as an alternative to CFD. The channel flow capability allows less computationally rigorous engineering scale solutions for applications that do not need the higher fidelity solution afforded by CFD. Further details on COBRA-TF will be found in later issues of *CASL Tech Notes*.

More information on CASL's thermal-hydraulics modeling strategy and the methods implemented within CASL's Hydra-TH code are available at CASL-I-2012-0055-000 and CASL-U-2012-0163-000, respectively.

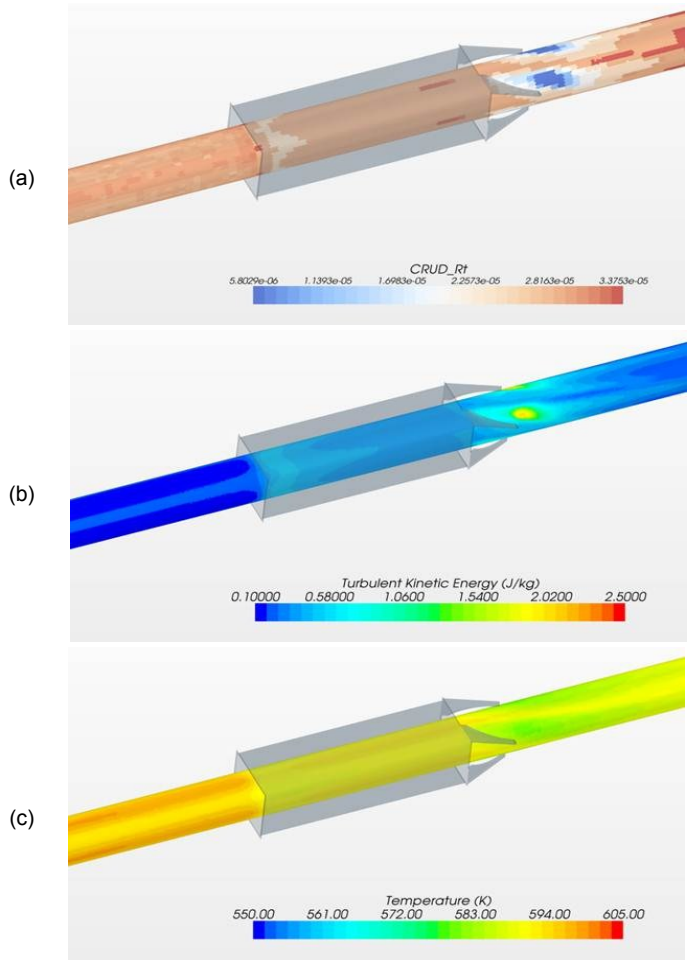

Fig. 7. (a) Crud thermal resistance [m^2K/W], (b) Turbulent kinetic energy, (c) Cladding temperature—simulation with MAMBA refined mesh at time t=80 days.

About CASL

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