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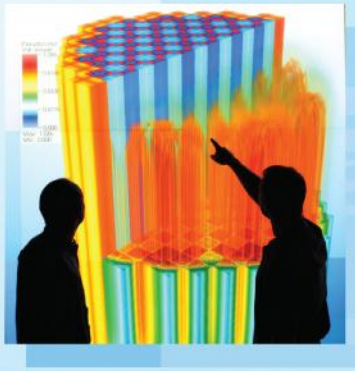

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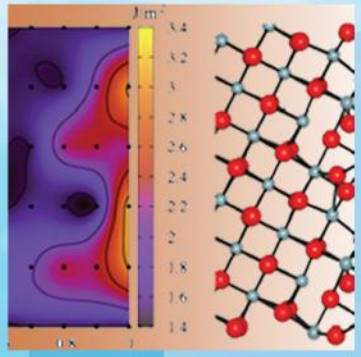

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CASL L1 Milestone Report: CASL.P4.01, Sensitivity and Uncertainty Analysis for CIPS with VIPRE-W and BOA

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CASL L1 Milestone Report: CASL.P4.01, Sensitivity and Uncertainty Analysis for CIPS with VIPRE-W and BOA

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Abstract

The CASL Level 1 Milestone CASL.P4.01, successfully completed in December 2011, aimed to "conduct, using methodologies integrated into VERA, a detailed sensitivity analysis and uncertainty quantification of a crud-relevant problem with baseline VERA capabilities (ANC/VIPRE-W/BOA)." The VUQ focus area led this effort, in partnership with AMA, and with support from VRI. DAKOTA was coupled to existing VIPRE-W thermal-hydraulics and BOA crud/boron deposit simulations representing a pressurized water reactor (PWR) that previously experienced crud-induced power shift (CIPS). This work supports understanding of CIPS by exploring the sensitivity and uncertainty in BOA outputs with respect to uncertain operating and model parameters. The studies focused on sensitivity and uncertainty of CIPS indicators calculated by the current version of the BOA code used in the industry. This report summarizes work coupling the software tools, characterizing uncertainties, and analyzing the results of iterative sensitivity and uncertainty studies. Challenges with this kind of analysis are identified to inform follow-on research goals and VERA development targeting crud-related challenge problems.

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The work is part of a cross-focus area CASL effort involving its VUQ, VRI, and AMA program elements. It benefitted from coordinating support by Jim Stewart (VUQ/SNL) and Zeses Karoutas (AMA/Westinghouse). Paul Turinsky (NCSU) provided technical review and guidance during execution, while Jeff Banta and Doug Kothe (ORNL) provided administrative oversight.

This sensitivity and uncertainty demonstration study relied heavily on problem statements, models, data, and technical guidance provided by Westinghouse Electric Company LLC. The authors thank Southern Nuclear Company for agreeing to share plant crud measurement data used in studies supporting this report. Dennis Hussey and Kenny Epperson (EPRI) and John Westacott (CSAI) consulted on BOA parameters, usage, and challenges. VRI staff including Chris Baker (ORNL) and Noel Belcourt (SNL) assisted with code and input example compilation and access. Keith Dalbey, Mike Eldred, and Laura Swiler (SNL) assisted with running and analyzing computational studies. Brian Williams (LANL) analyzed available plant measurement data. Computational hardware and support was provided by SNL.

The authors thank the reviewers of this report, including many of those noted above.

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NOMENCLATURE

AMA	Advanced Modeling Applications (CASL technical focus area)
AOA	Axial offset anomaly
BOA	Boron-induced offset anomaly
CASL	Consortium for Advanced Simulation of LWRs
CIPS	Crud-induced power shift
CSAI	Computer Simulation & Analysis, Inc.
DAKOTA	Design and Analysis ToolKit for Optimization and Terascale Applications
DOE	Department of Energy
EPRI	Electric Power Research Institute
LANL	Los Alamos National Laboratory
LWR	Light water reactor
m-dot-e	Mass evaporation rate
NCSU	North Carolina State University
ORNL	Oak Ridge National Laboratory
PWR	Pressurized water reactor
SA	Sensitivity analysis
SNL	Sandia National Laboratories
UQ	Uncertainty quantification
TVA	Tennessee Valley Authority
VBD	Variance-based decomposition
VERA	Virtual Environment for Reactor Applications
VIPRE-W	Thermal hydraulics subchannel simulator code (Fortran)
VRI	Virtual Reactor Integration (CASL technical focus area)
VUQ	Validation and Uncertainty Quantification (CASL technical focus area)
Westinghouse	Westinghouse Electric Company LLC

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1. EXECUTIVE SUMMARY

Analysis and improved scientific understanding of crud formation on nuclear fuel rod surfaces and its impact on operating light water reactors (LWRs), such as crud-induced power shift (CIPS), are central to the mission of the Consortium for Advanced Simulation of LWRs (CASL) DOE Energy Innovation Hub. The CASL Level 1 Milestone CASL.P4.01, executed jointly by the VUQ and AMA focus areas, with support from VRI, directly supports better understanding of these reactor performance-critical phenomena by performing DAKOTA studies on coupled thermal-hydraulics / crud / boron deposit simulations of an operating commercial reactor that previously experienced CIPS.

CIPS, previously referred to as axial offset anomaly (AOA), is an unexpected shift in axial power towards the reactor core inlet, resulting from crud buildup on the fuel rods during operation. Corrosion of the reactor coolant system (RCS) surfaces releases nickel and iron into the coolant. The nickel and iron are deposited in the upper spans of high heat flux assemblies where sub-cooled boiling occurs. Boric acid and lithium hydroxide concentrate in the porous crud and boron precipitates when sufficiently concentrated. The boron dissolves as sub-cooled boiling is reduced and is returned to the coolant along with lithium. CIPS is most common in PWR cores with increased fuel thermal duty, as a result of power uprate or other plant changes.

The principal deliverable of this milestone is a capability demonstration of global sensitivity and uncertainty analysis of thermal-hydraulic and crud/boron deposit simulations using the baseline VERA codes for a Westinghouse-designed four-loop pressurized water reactor (PWR). DAKOTA algorithms assessed the influence of thermal hydraulic and crud model parameters on crud and boron deposit predictors for a representative plant. Sensitivity analysis (SA) determined the influence of parameters to rank their relative importance, while uncertainty quantification (UQ) assessed the mean and variance of the crud-related metrics, with respect to input parameter uncertainties. This is the most extensive study conducted to-date with these two coupled simulation codes.

The team performed the following work:

- selected a Westinghouse-designed operating nuclear reactor which experienced CIPS and for which crud-related measurement data and simulation models were readily available;
- prepared input files (models) for baseline VERA VIPRE-W and BOA codes to simulate thermal-hydraulics and crud and boron deposits, including templating them to accept DAKOTA parameter variations;
- chose uncertain code input parameters, characterized prior information on their uncertainties, and created corresponding DAKOTA input files for various SA and UQ methods;
- held extensive discussions to prioritize study resources, understand physical phenomena, and triage code robustness issues;
- developed a (loose-coupled) workflow using VERA modules to robustly execute the physics codes, potentially over multiple cycles and burn-up steps, and perform post-processing to extract metrics;
- executed DAKOTA to perform demonstration sensitivity and uncertainty studies; and

- summarized and discussed the results, elucidating challenges encountered and recommendations for further study.

Key outcomes (see details in Sections 5 and 6) of this work include:

- creation of a workflow to execute VIPRE-W coupled to BOA across multiple cycles in iterative parametric studies with DAKOTA;
- identification of the thermal-hydraulic and crud modeling parameters most influential on CIPS-related BOA outputs, including potential nonlinear relationships;
- statistical quantification of the uncertainty they induce in crud predictors such as boron mass and crud thickness;
- enumeration of challenges (and possible mitigation strategies) with characterizing multivariate uncertainties in physically meaningful ways, highlighting the need for additional calibration and validation data, and coupled code robustness to parameter variations; and
- amplifying the perceived importance of out-of-core crud source terms such as corrosion product release factors in predicting CIPS.

This milestone paves the way for upcoming CASL developments, including, but not limited to:

- more sophisticated analysis workflows and close-coupling of VUQ and physics modeling tools within VERA;
- sensitivity, uncertainty, calibration, and validation analysis with fully-coupled neutronics, thermal-hydraulics, and crud models, including next-generation simulation tools that CASL will produce and/or integrate;
- use of DAKOTA to calibrate BOA crud prediction models to data from various plants in contrast to previous manual processes; and
- prioritizing the development of emerging CASL physics codes to better understand CIPS in particular and fuel performance/reliability risk assessment in general.

In turn, this report summarizes simulations and responses of interest, the DAKOTA and simulation infrastructure used, the parameters studied and their characterizations of uncertainty, and prototypical results for global sensitivity and uncertainty, including challenges applying them in this context. Perhaps the most important outcome of this effort is the resulting set of lessons learned which will expedite future VUQ-related work for CIPS, motivate fundamental physics model development, and inform targeted data collection.

NOTE: *This report is a high-level summary and not intended to detail all the computational experiments conducted or corresponding results. Additional details are available on request from the authors.*

2. TARGET PLANT, MODELS, AND METRICS

In order to better understand the CIPS challenge problem, this milestone study focused on a Westinghouse-designed PWR "Plant C," which experienced CIPS in its previous operating cycles. This is a four-loop PWR using the Westinghouse 17x17 VANTAGE 5 (V5) fuel design with a fuel rod outside diameter of 0.360 inches (9.14 mm) and a reference active heated length of twelve feet (365.8 cm). The V5 fuel design contains six mixing vane grid spacers with an additional three Intermediate Flow Mixer grids for enhanced thermal performance. For this Plant C, cycles 11 through 15 are the object of study as they include a period with CIPS occurrence.

Available data also motivated the selection of Plant C, as it will enable follow-on calibration and validation studies. As part of the effort to understand CIPS occurrences, the Plant C core crud deposits were investigated. During reactor refueling, several fuel assemblies were scraped and full face videos of every assembly were taken. Each fuel assembly was video camera-inspected from top to bottom on all four faces after removal from the up-ender during the off-loading process. Crud coverage on each fuel assembly was estimated from the video images and a "crud index" value of 0 through 10 assigned, with 10 representing 100 percent coverage. Some crud samples were collected from a twice-burned fuel assembly and three once-burned assemblies for detailed analyses including scanning electron microscopy, phase composition by X-ray diffraction, and gamma spectroscopy [1]. In future studies, the data collected from those measurements will be compared to the same metrics considered in this study to adjust and/or assess agreement between models and reality.

Earlier CASL studies [2, 3] focused solely on thermal-hydraulics calculations with VIPRE-W for "Plant A" and "Plant B" models. In these, mass evaporation rate (m-dot-e) as calculated by VIPRE-W was used to calculate a "boiling index" indicating the percentage of each grid span experiencing boiling. Comparisons between boiling index and the corresponding crud index calculated from post-cycle visual examination data were made for several assemblies, under the assumption that the boiling index should be consistent with the crud index. In contrast, the present study couples VIPRE-W to Electric Power Research Institute's (EPRI's) Boron-induced Offset Anomaly (BOA) Risk Assessment Tool to calculate crud and boron deposits on the fuel rods as they are more direct predictors of CIPS. However, in these, the spatial element was suppressed, focusing instead on summary output for each cycle considered.

Consistent with the current practice for CIPS risk assessments in the industry, simulations for the four-loop PWR core were based on the quarter core geometry and computational grid shown in Figure 1, with 193 flow channels (shown) and 93 nodes with a nodal length of about 50 mm (2 inches) in the axial direction (not shown). Each flow channel represents one quarter of a fuel assembly. Feedback to neutronics and its subsequent influence on the VIPRE-W and BOA calculations is not considered in this study.

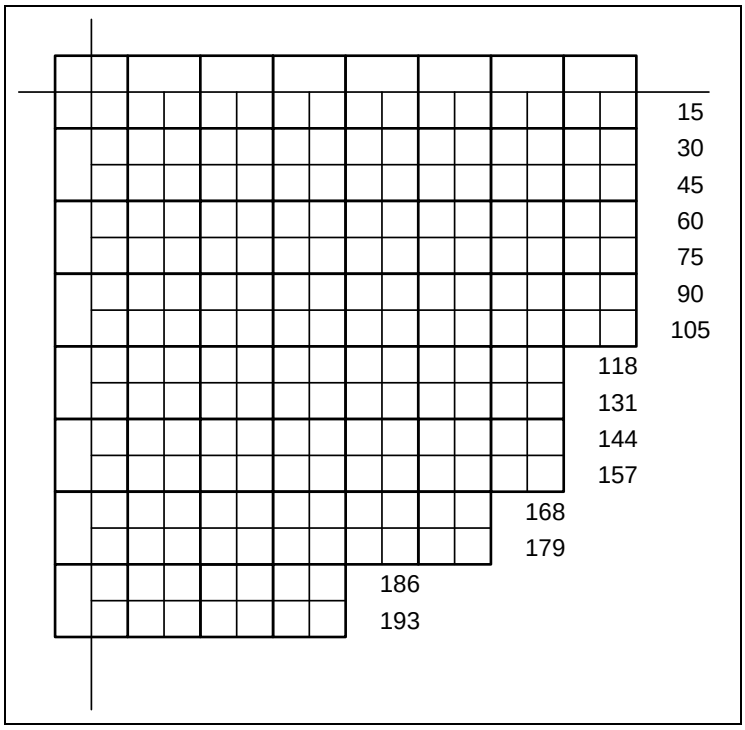

Figure 1. VIPRE-W quarter core geometry and channel layout.

VIPRE-W Simulations

Thermal-hydraulics calculations were performed with VIPRE-W, a Westinghouse version of the VIPRE-01 code. VIPRE-01 is a thermal-hydraulic subchannel code based on the COBRA codes developed by Pacific Northwest National Laboratories under sponsorship of EPRI [4]. VIPRE-W contains enhancements for PWR applications, including the mass evaporation and grid spacer heat transfer models required for CIPS risk assessment.

Baseline VIPRE-W input decks for Plant C cycles 11—15 were furnished by Westinghouse [5]. The number of burn-up steps used varies from cycle to cycle, with early steps based on standard MWD/MTU increments needed to equilibrate crucial elements/isotopes, and final steps depending on cycle length, as shown in Table 1. After initial testing and discussions, the inputs were modified to remove the proprietary WRB-2 DNB correlation so the models would run with the CASL VERA version of the VIPRE-W code. The VIPRE-W input decks are consistent with those previously used for Plant C CIPS risk assessments.

Table 1. Burn-up steps used in VIPRE-W simulations for each cycle.

Cycle	Burn-up Steps (MWD/MTU)
11	150, 1000, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 12000, 14000, 16000, 18000, 20000, 21660
12	150, 1000, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 12000, 14000, 16000, 18000, 20000, 21100, 21610
13	150, 1000, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 12000, 14000, 16000, 18000, 20000, 21000, 22265
14	150, 1000, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 12000, 14000, 16000, 18000, 20000, 20450, 21238
15	150, 1000, 2000, 3000, 4000, 5000, 6000, 8000, 10000, 12000, 14000, 16000, 18000, 20000, 21500, 22300, 23000

BOA Simulations

The Boron-induced Offset Anomaly (BOA) Risk Assessment Tool [6] simulates the process leading to CIPS, including crud deposition on the fuel cladding surfaces and precipitation of boron within the crud. The BOA code uses thermal/hydraulic conditions determined by VIPRE-W, together with models for corrosion product release, transport, and deposition, to predict crud deposition on the core. If crud deposits become sufficiently thick, boron compounds are predicted to deposit within the crud layer. BOA seeks to help the industry to characterize crud deposition and risk of AOA when doing core reload designs and to evaluate the potential effects in a reactor core when AOA has occurred. For instance, core boron mass and crud thickness predicted by BOA are key indicators for CIPS.

Crud-related predictions, based on the output VIPRE-W thermal-hydraulic conditions, were calculated with BOA Version 3.0 (released December 2010), using modified versions of baseline BOA input decks for Plant C cycles 11—15 furnished by Westinghouse [5]. Some fuel cycles where trips occurred were split into two parts for calculation purposes, therefore data and inputs used include restart data from cycle 10, single-part inputs for cycles 12, 14, and 15, and two-part inputs for cycles 11 and 13.

BOA calculates metrics such as boron mass, nickel and iron concentrations, and crud thickness, as important predictors for a CIPS occurrence. While BOA calculates these at every node in the computational domain described above, this study focuses on metrics integrated over both space and time. Table 2 summarizes the response metrics of interest in this study, determined through discussion among SNL, Westinghouse, and EPRI experts. Except as indicated, all metrics were derived from post-processing BOA's .out file. The abbreviations indicated are used in DAKOTA/BOA interfaces and will be used in presenting results.

Table 2. Integral response metrics derived from BOA output.

Description	Units	Abbreviation in Interfaces/Results
End-of-cycle (EOC) maximum core boron mass	lbm	BoronMass
EOC maximum crud thickness	mils	CrudThick
EOC nickel/iron ratio	1	NiFeRatio
EOC nickel metal mass	lbm	NiMetalMass
Median nickel across cycle	ppb	MedianNi
Median iron across cycle	ppb	MedianFe
EOC/BOC crud ratio (.bor file)	1	CrudFraction

3. DAKOTA AND SIMULATION WORKFLOW

The milestone studies used DAKOTA 5.1 to perform both single and joint parameter variation to assess the effect of input parameters (over their whole range of inputs) on response metrics output by the forward-coupled physics. This section briefly reiterates DAKOTA's capabilities and how it interfaces to a simulation, describes the workflow developed for these studies, and mentions the algorithms applied. A slightly more detailed overview of these approaches is available in [2], with extensive details in the DAKOTA documentation.

DAKOTA Overview and Algorithms Used

DAKOTA (Design and Analysis ToolKit for Optimization and Terascale Applications) is a freely available, SNL-developed software package for sensitivity analysis, optimization, uncertainty quantification, and calibration with black-box computational models [7]. DAKOTA provides a flexible, extensible interface to any analysis code, includes both established and research algorithms designed to handle challenges with science and engineering models, and manages parallelism for concurrent simulations (hence many concurrent executions of VIPRE-W and BOA were possible for this study). DAKOTA strategies support mixed deterministic/probabilistic analyses and other hybrid algorithms.

The present work leveraged DAKOTA's centered parameter study and Latin hypercube sampling (LHS, in Monte Carlo mode) algorithms to perform global sensitivity and uncertainty analysis. The parameter study offers a glimpse at the overall sensitivity and smoothness of the model by performing single parameter variations in terms of deviation from their nominal values, over the whole admissible range. For global sensitivity analysis, we consider the LHS-generated points, together with partial correlation coefficients and scatter plots. For uncertainty quantification (UQ), we examine sample means, standard deviations, and empirical output histograms from the raw sample sets.

Simulation Workflow

To perform optimization, uncertainty quantification, or sensitivity analysis in a loose-coupled or "black-box" mode, DAKOTA iteratively writes parameter files, invokes a script to run the computational model, and collects resulting responses from a results file. This overall execution process is depicted in

Figure 2. Typically application codes like VIPRE-W and BOA do not directly accept DAKOTA parameters or extract derived responses to produce DAKOTA-formatted results files, requiring a wrapper script or other executable to coordinate their execution. For most applications with text-based input and output, developing such a workflow typically requires from a few hours to a week of labor, where most of the variability is due to difficulty deriving desired responses from raw code output. Nuances of code execution, input/output formats, and robustness with respect to parameter variations (automated warning and error detection) can also make this exercise more demanding and time consuming. Once application-specific scripts are implemented, various DAKOTA methods can be applied with minor modification to the DAKOTA input file.

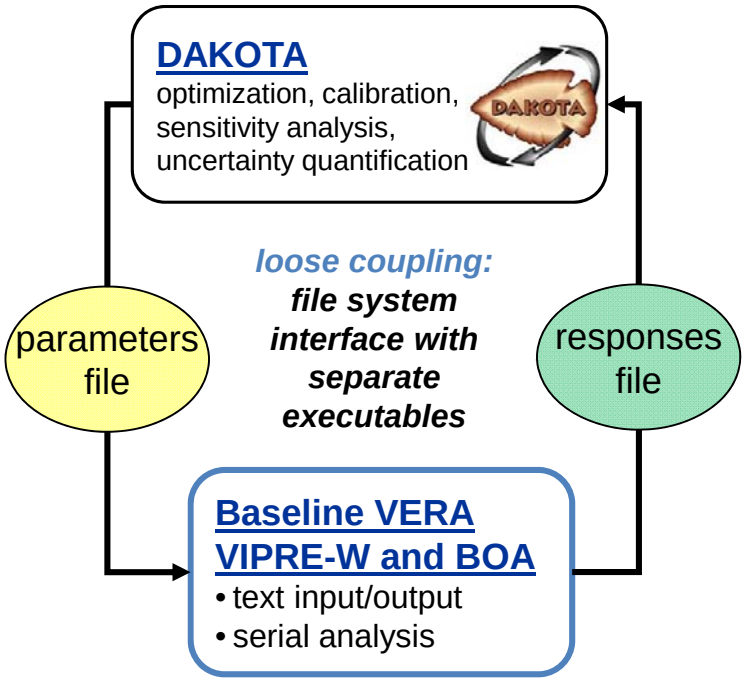

Figure 2. Loose ("black-box") coupling of DAKOTA to VIPRE-W and BOA.

A more detailed view of a DAKOTA workflow is shown in Figure 3. The components in the dashed box, which include integrating parameters into the simulation, running the code(s), and post-processing the output, are unique to a particular application interface. The work for this milestone included developing a modular Python-based workflow to implement this part of the workflow. This infrastructure coordinates running VIPRE-W and BOA across multiple cycles, feeding data forward as needed. Script elements developed in previous CASL work [2] were matured into Python script modules with the following key features:

- selection of which cycles to iterate over and run;
- creation of directories in which to cloister each simulation run, including (1) efficiently linking static files, e.g., restart files, (2) inserting DAKOTA parameters with dprepro, or (3) copying files specific to each evaluation;
- for each cycle,
    - optionally run VIPRE-W for a sequence of burn-up steps to generate necessary .aoa data, then
    - optionally run BOA (either using static or freshly generated output .aoa files, depending on whether there are VIPRE-W parameter variations), potentially for multiple parts within a cycle,

  which permits studying just BOA or the coupled code system;
- ability to extract metrics from BOA either (1) aggregating .out data over a cycle, (2) parsing .out data at the end of a cycle, or (3) using the Boron summary (.bor) file;
- capture warnings in BOA output and communicate them to DAKOTA; and
- numerous options for controlling verbosity, persistence of files, and debugging.

While this study used Python scripts to link DAKOTA and couple VIPRE-W to BOA, CASL VUQ and VRI are coordinating to tightly link DAKOTA with physics codes in VERA and

coordinate overall workflows with VERA workflow tools. We anticipate that creation and execution of similar studies will get increasingly simpler and efficient.

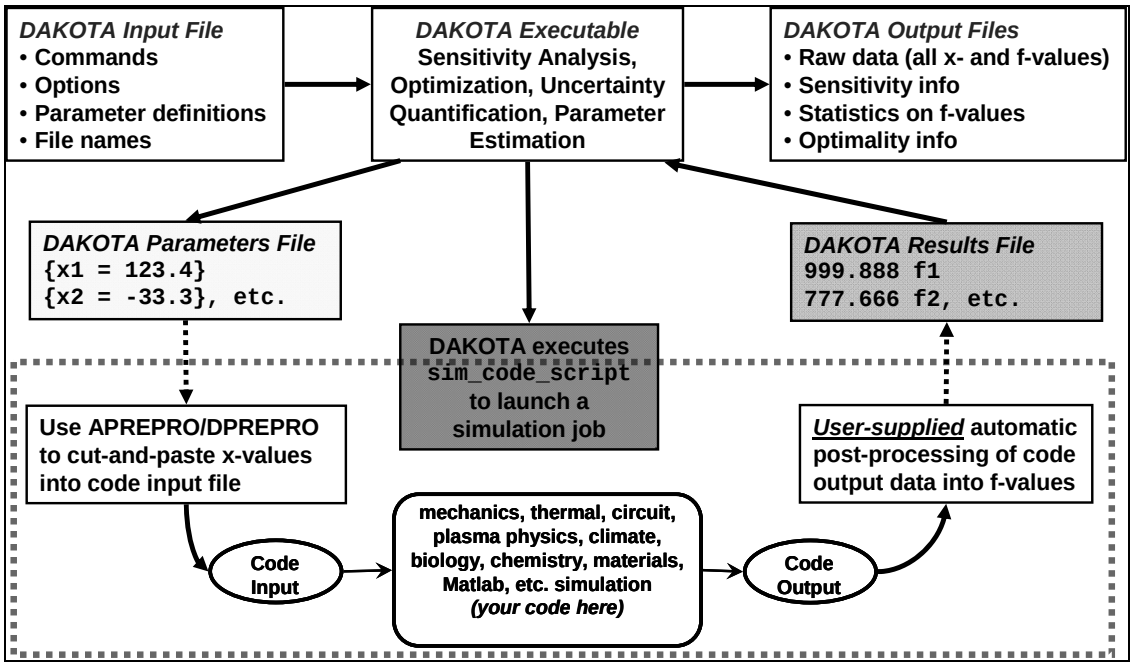

Figure 3. DAKOTA workflow details and analysis driver script for a generic application.

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4. UNCERTAINTY CHARACTERIZATIONS AND DAKOTA SPECIFICATIONS

This section summarizes the model input parameters used in the sensitivity analysis and uncertainty quantification studies, including their nominal values and uncertainties. The mapping from simulation code terminology to DAKOTA parameter names is given in Table 3. The DAKOTA names are used in the analysis process for automatic parameter manipulation and post processing.

Table 3. Summary of parameters considered.

Code applied to	Parameter Description	DAKOTA Name	Name in Results
VIPRE-W	(multiplier on) fuel assembly power	PowerMult	Power
	(multiplier on) coolant flow	FlowMult	Flow
	inlet temperature (°F)	Temp	Temp
	system pressurizer pressure (psia)	Press	Press
VIPRE-W/ BOA	lead coefficient of Dittus-Bolter correlation*	DBC	DBC
BOA	k_a: soluble precipitation rate constant for Ni metal and NiO	PRCKA	PRCKA
	k_b soluble precipitation rate constant for $NiFe_2O_4$	PRCKB	PRCKB
	k_{dX}: particle Y deposition constant for non-boiling surfaces; PDRNX†	PDRN	PDRN
	k_{dX}: particle Y deposition constant for boiling surfaces; PDRBX†	PDRB	PDRB
	k_r: particle release constant for non-boiling core surfaces	CKNB	CKNB
	k_{r1}: particle release constant for boiling surfaces (CKBL = CKBLmult*CKNB)	CKBLmult	CKBL
	k_{r2}: particle release constant for out of core surfaces (hot/cold leg & SG)	CKSG	CKSG
	crud mapping multiplier	FM	FM
	Ni release fraction applied to Ni corrosion rate, CREL	RFNI	n/a
	Fe release fraction applied to Fe corrosion rate, CRELFE	RFFE	n/a

**For these studies, DBC was only varied in BOA, as it recalculates the boiling and fuel rod heat transfer coefficients. In a transient study it would be necessary to map it into both simulation codes.*

†A single control PDRN adjusted deposition for X = {1, 2, 3}, corresponding to particles Y = {Ni, $NiFe_2O_4$, NiO}; similar for PDRB.

Specified Uncertainties

Table 4 contains representative thermal-hydraulic uncertainty ranges to be considered, similar to those provided by Westinghouse for Plant C [5]. The actual uncertainty characterizations used in the computational studies are based on rigorous design and data analysis for this plant. Previous work [2] indicated these variables have the strongest influence on mass evaporation rate. Based on that work and Westinghouse judgment, less influential inputs are omitted from the present study. Power and flow are treated with multipliers instead of absolute values as the nominal values differ for the five operational cycles considered. While nominal temperature and pressure

vary slightly among cycles, their typical values and variation is considerably less than the uncertainty prescribed in Table 4, so they were treated in an absolute sense.

Table 5 indicates the crud deposition and release variables to be considered, using names from the BOA manual [6], which also describes some of the solution principles and formulations. A single control variable PDRN mapped to BOA's PDRN1—3 in the studies and similar for PDRB to PDRB1—3. The effect of parameter CKBL was represented as a multiplier on the realization of CKNB for a given evaluation in the study (CKBL = CKBLmult*CKNB). Finally, Table 6 shows the corrosion product uncertainties used, although for reasons discussed in Section 5.1, results for RFNI and RFFE are not included. The crud model uncertainty characterizations in these tables are based on expert judgment and treated as uniform in the specified intervals.

Table 4. Thermal-hydraulic variables with specified uncertainties (notional).

Parameter	Range	Calibrated	Uncertainty	Continuous	VIPRE-W Input
Fuel Assembly Power (Fraction of Core Average)	0.15 – 1.446*	No	about 6% normal	Yes	OPER.5 (for simplicity)
Coolant Flow (gpm)	0.973 – 1.026*	No	< 3% normal	Yes	OPER.5
Inlet Temperature (^oF)	551.4 – 562.3	No	About 5 ^oF normal	Yes	OPER.5
System Pressure (psia)	2220 – 2307.4	No	< 40 psi normal	Yes	OPER.5
Lead Coefficient of Dittus-Bolter Correlation	0.019 – 0.033	Yes	N/A	Yes	CORR.7

** Specified range is fraction of nominal.*

Table 5. Crud deposition and release variables with specified uncertainties.

Parameter	Nominal Value	Min	Max	Comment
PRCKA, Ni^o, NiO	2.74E-5	-25%	+25%	Soluble precipitation rate constant
PRCKB, $NiFe_2O_4$	1.51E-6	-25%	+25%	Soluble precipitation rate constant
PDRN1, Ni^o	1.0E-6	1.0E-7	2.0E-6	Particulate deposition, non-boiling region
PDRN2, NiO	1.0E-6	1.0E-7	2.0E-6	Particulate deposition, non-boiling region
PDRN3, $NiFe_2O_4$	1.0E-6	1.0E-7	2.0E-6	Particulate deposition, non-boiling region
PDRB1, Ni^o	1.0E-6	1.0E-7	2.0E-6	Particulate deposition in boiling region
PDRB2, NiO	1.0E-6	1.0E-7	2.0E-6	Particulate deposition in boiling region
PDRB3, $NiFe_2O_4$	1.0E-6	1.0E-7	2.0E-6	Particulate deposition in boiling region
CKNB	5.5E-8	5.5E-9	5.5E-7	Particulate release coefficient (core non-boiling)
CKBL	0.5*CKNB	0.3*CKNB	0.5*CKNB	Particulate release coefficient (core boiling)
CKSG	5.5E-8	5.5E-9	5.5E-7	Particulate release coefficient (out-of-core non-boiling)

Generally we expect PDRN1=PDRN2=PDRN3, and PDRB1=PDRB2=PDRB3

Table 6. Corrosion product variables with specified uncertainties

Parameter	Nominal Value	Min	Max	Comment
RFNI	0.519	0.7*RFNI	1.3*RFNI	A600 Release fraction of Ni from SG tubing
RFFE	0.534	0.7*RFNI	1.3*RFNI	Release fraction of Fe from SS piping
FM	0.7	0.5	0.9	Reinsert Core Crud Fraction

Effective DAKOTA Distributions

The following conventions guided the translation of the above Westinghouse-provided uncertainty specifications into uncertain distributions for use with DAKOTA:

- Reactor operating parameters were treated with truncated normal distributions, with mean equal to the bias-adjusted nominal value (from the input file) and standard deviation equal to half the specified uncertainty value. The distribution was bounded (truncated) at bias-adjusted nominal ± uncertainty, unless the bound exceeded the provided parameter ranges, in which case the more restrictive range bound took precedence.
- Cases with prescribed uncertainty, with only minimum and maximum values, were treated as uniform over the provided range of uncertainty.

Table 7. Resulting DAKOTA normal distributions (notional).

Parameter	Mean	Standard Deviation	Lower Bound (truncation)	Upper Bound (truncation)
PowerMult	1.0	0.03	0.94	1.06
FlowMult	1.0	<0.015	>0.97	<1.03
Temp	557.1	2.5	552.1	562.1
Press	2257.4	<20.0	>2217.4	<2297.4

Table 8. Resulting DAKOTA uniform distributions.

Parameter	Lower Bound	Upper Bound
DBC	0.019	0.033
PRCKA	2.0550e-05	3.4250e-05
PRCKB	1.1325e-06	1.8875e-06
PDRN	1.0e-7	2.0e-6
PDRB	1.0e-7	2.0e-6
CKNB	5.5e-9	5.5e-7
CKBLmult	0.3	0.5
CKSG	5.5e-9	5.5e-7
FM	0.5	0.9

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CASL-U-2011-0171-000

5. SENSITIVITY AND UNCERTAINTY RESULTS

This section summarizes exploratory Plant C studies conducted with DAKOTA, VIPRE-W, and BOA using the above uncertainty characterizations and workflow management scripts. A total of thirteen parameters and seven response functions from Table 2 (for each cycle for a total of 35 responses) were studied to demonstrate the approach. Challenges with code robustness to parameter variations are described, and overall recommendations for follow-on studies enumerated. All studies were conducted on the Redsky compute cluster [8] at Sandia National Laboratories. One execution of the coupled VIPRE-W/BOA workflow for all five cycles takes an average of 45 minutes on one CPU, so the 1300 sample study discussed below required nearly 1,000 CPU hours.

5.1. Initial Challenges Discovered

In the early phases of this work we verified the execution of VIPRE-W and BOA using the nominal input conditions and the outputs against previous calculations conducted by Westinghouse. This resulted in small modifications such as the VIPRE-W correlation model and an assessment of nominal run times. Westinghouse and SNL coordinated to verify parameter insert locations and extraction of response metrics. Some of the challenges encountered during ramp-up are enumerated in this section.

Pressure Outside Table Limits
In initial exploratory runs, and later in coupled VIPRE-W/BOA runs, BOA reported that requested pressures were outside lookup table limits. We mitigated this by adjusting the BOA input so calculated steam tables spanned the range of operating pressures considered for VIPRE (specifically we adjusted the lower bound on pressure for the calculated table). However, in a more general setting, BOA's table lookup ranges (specified via lower bound and increment) might have to be automatically adapted to the realization of uncertain parameters to ensure success.

Treatment of Power and Flow
While a single nominal temperature and pressure well represented all five cycles of the baseline cases, the power and flow varied more across cycles. We decided to treat these parameters with a relative deviation from the nominal for a given cycle. In a more general case, each of these might have to be treated with a relative perturbation.

Creating Numerous Template Files
This study included a total of 80 VIPRE-W and seven BOA input files. While some automated creation of templates to accept DAKOTA parameters was possible, a better solution will be needed longer term. This could be addressed by VERA development plans which aim to standardize on a common input format among simulation codes, with appropriate translators.

Negative Mass Warnings from BOA
Perhaps the greatest challenge encountered was simulation robustness to joint parameter variations. A preliminary LHS study was conducted using only BOA over five cycles, with the

parameters listed in Table 5 and Table 6, excepting CKBL (its treatment as a multiplier was not yet agreed upon). Analysis of the results of this nine parameter, 900 sample study, together with guidance from EPRI about BOA warnings, revealed that DAKOTA parameter variations often yielded errant simulations, with BOA returning negative mass warnings, i.e., the balance laws could not be satisfied for the amounts of nickel and iron in the system.

When encountering this warning, a typical calibration workflow dictates adjusting input variable SNI, which parameterizes the amounts of nickel and iron in the compound used in the deposition model. Specifically, s = SNI in $Ni_sFe_{(3-s)}O_4$, which permits the compound to vary from 0.0 (magnetite, Fe_3O_4) to 1.0 (nickel ferrite, $NiFe_2O_4$) [6]. This led to a sequence of DAKOTA/BOA calculations varying all eleven BOA parameters from Table 5 and Table 6, with SNI ranging from 0.8 to 0.1 in 0.1 increments. For each SNI value, 550 LHS samples were run. These studies still contained a large percentage of simulation "failures" (warnings), as shown in Table 9, where:

- **WS** indicates number of samples out of 550 containing any warning;
- **TW** indicates total number of times negative mass warning appeared in output; and
- **LB** indicates the lower bound on RFNI/RFFE ratio that would yield no warnings

Table 9. BOA warnings encountered for various values of SNI.

	Cycle 11			Cycle 12			Cycle 13			Cycle 14			Cycle 15		
SNI	**WS**	**TW**	**LB**	**WS**	**TW**	**LB**	**WS**	**TW**	**LB**	**WS**	**TW**	**LB**	**WS**	**TW**	**LB**
0.8	*3*	*179*	*0.8*	*187*	*8888*	*1.3*	*44*	*1558*	*1.2*	*178*	*10308*	*1.5*	*106*	*7220*	*1.5*
0.7	58	812	1.1	120	4260	1.2	44	4156	1.1	116	5306	1.6	69	3072	1.6
0.6	22	228	1.0	63	1324	1.1	15	991	1.0	76	2147	1.5	47	890	1.5
0.5	8	88	0.8	22	244	0.9	6	143	0.7	52	609	1.6	36	189	1.6
0.4	1	8	0.6	7	14	1.2	0	0	0	45	244	1.5	35	156	1.4
0.3	2	22	0.9	13	44	1.0	0	0	0	47	303	1.3	35	192	1.3
0.2	3	26	0.8	4	4	0.7	0	0	0	44	270	1.5	35	165	1.5
0.1	0	0	0.0	0	0	0.0	0	0	0	45	293	1.6	35	164	1.6

Note: for SNI = 0.8, warnings were only calculated over the second part of multi-part cycles (cycles 11 and 13), so the warning counts are almost surely underestimated.

Analysis of the resulting data did not reveal correlation of failures with any single parameter, nor with the ratio of nickel to iron released (although reducing the overall ranges of the parameters, especially DBC, or constraining the RFNI/RFFE ratio appeared promising in limiting failures). The joint variation of all the parameters in a global sensitivity study seemed to cause the failures. Further discussion led to a decision to omit the RNFI and RFFE variables from this study, which resulted in a dramatic improvement in percentage of completed runs for later cycles. Given the likely importance of these variables, they will require treatment in a future study.

These studies revealed a need for more robust post-processing of the BOA output to check for this warning. For this study, the scripts check only for negative mass warnings; in the future, other warnings and errors should be checked. Due to error detection, the results for the 1300 LHS samples below (taken over four VIPRE-W and the nine remaining BOA parameters) omit any "failed" samples, leveraging DAKOTA's failure detection mechanism.

Table 10 shows the number of failed samples for each cycle. Since future cycles depend on boron and crud from previous cycles, the analysis flow is aborted whenever a warning is encountered and all remaining cycles for that sample are discarded.

Table 10. Failed evaluations for each cycle (of 1300 evaluations).

Cycle	11	12	13	14	15
Failed Evaluations	145	285	285	375	375

5.2. Single Parameter Variations

Varying one parameter at a time, fixing all others at their nominal values, is often helpful in the early exploration phase of sensitivity and uncertainty studies. It offers insight on the robustness of the simulation code, the smoothness of the outputs, and the range of variability due to single factors. DAKOTA's "centered parameter study" exercises the simulation in this way, as depicted in Figure 4 for a problem with two variables d1 and d2, with two steps in each of the positive and negative coordinate directions. For the example in this diagram, DAKOTA's parallel scheduling could potentially execute the simulation code at all nine points simultaneously.

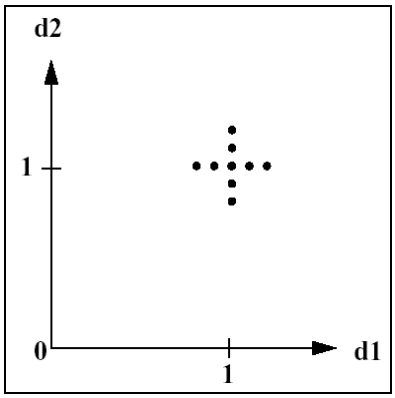

Figure 4. Diagram of centered parameter study.

Plant C centered parameter studies were conducted using the ranges of thirteen parameters as shown in Table 7 and Table 8, with the nominal value for each parameter placed at the midpoint of the specified lower/upper bounds. Each parameter was varied over ten negative and ten positive increments. Example results for the end of cycle maximum crud thickness for cycle 11 are shown in Figure 5. From this, observe:

- most, but not all of the single parameter variations induce smooth variations in the response;
- some appear to have a nonlinear effect on the response, though many have a linear effect; and
- further investigation of parameters like PowerMult, DBC, and CKNB may be necessary.

From this parameter study we also gain insight into the simulation failures. For cycle 11, all of the parameter variations over the complete range were successful, for all response metrics. However, in cycle 12 (and therefore in all following cycles), there are problems with PowerMult

≤ 0.9580 (4 smallest values considered), Temp ≤ 552.6 (2 smallest values considered), and DBC ≥ 0.0309 (4 largest values considered). This is demonstrated in Figure 6 for boron mass in cycle 12. Further, starting in cycle 14, CKNB ≥ 5.2278e-07 (2 largest values considered) is problematic (not shown).

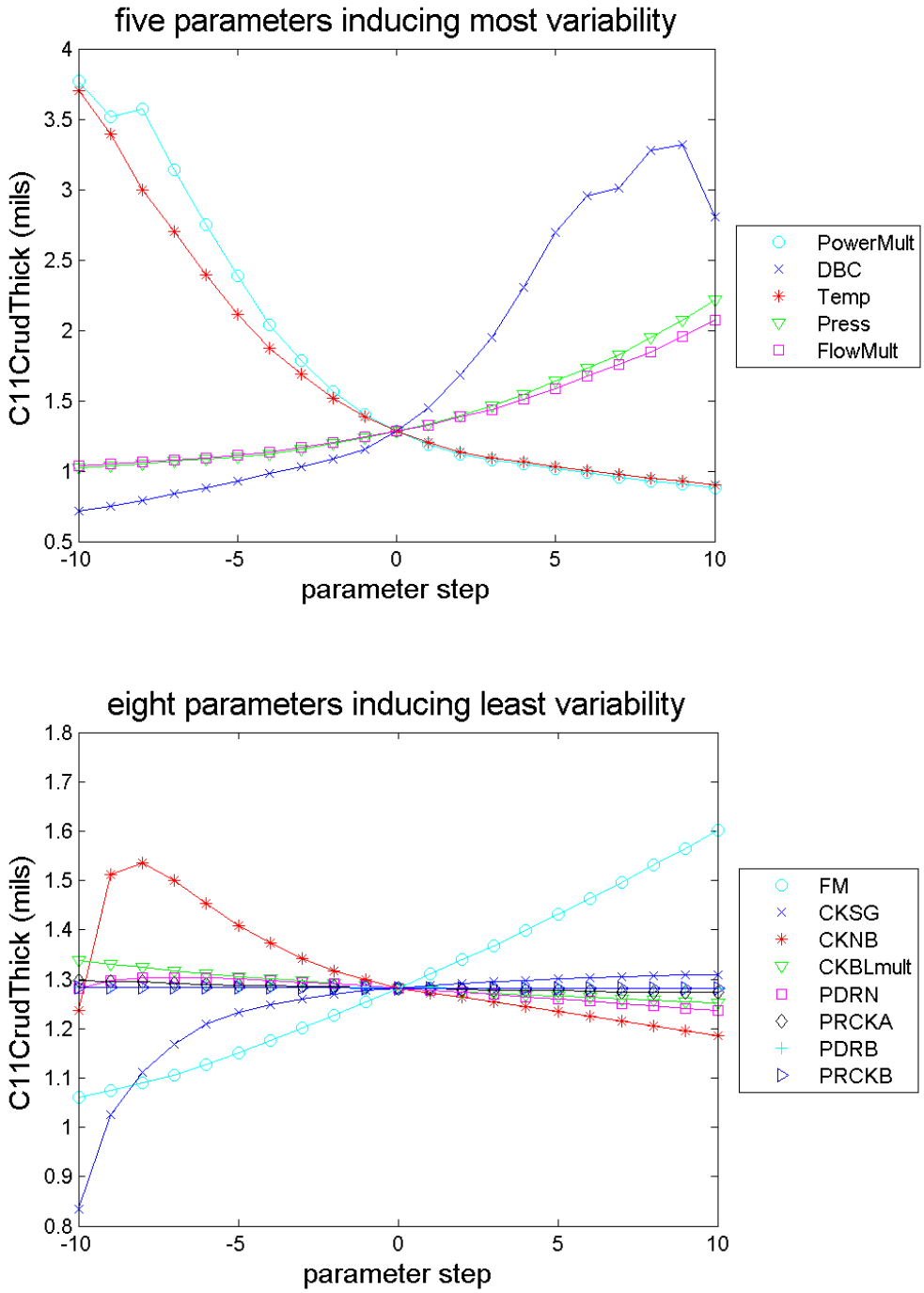

Figure 5. Univariate parameter sensitivities for end of cycle 11 crud thickness (mils).

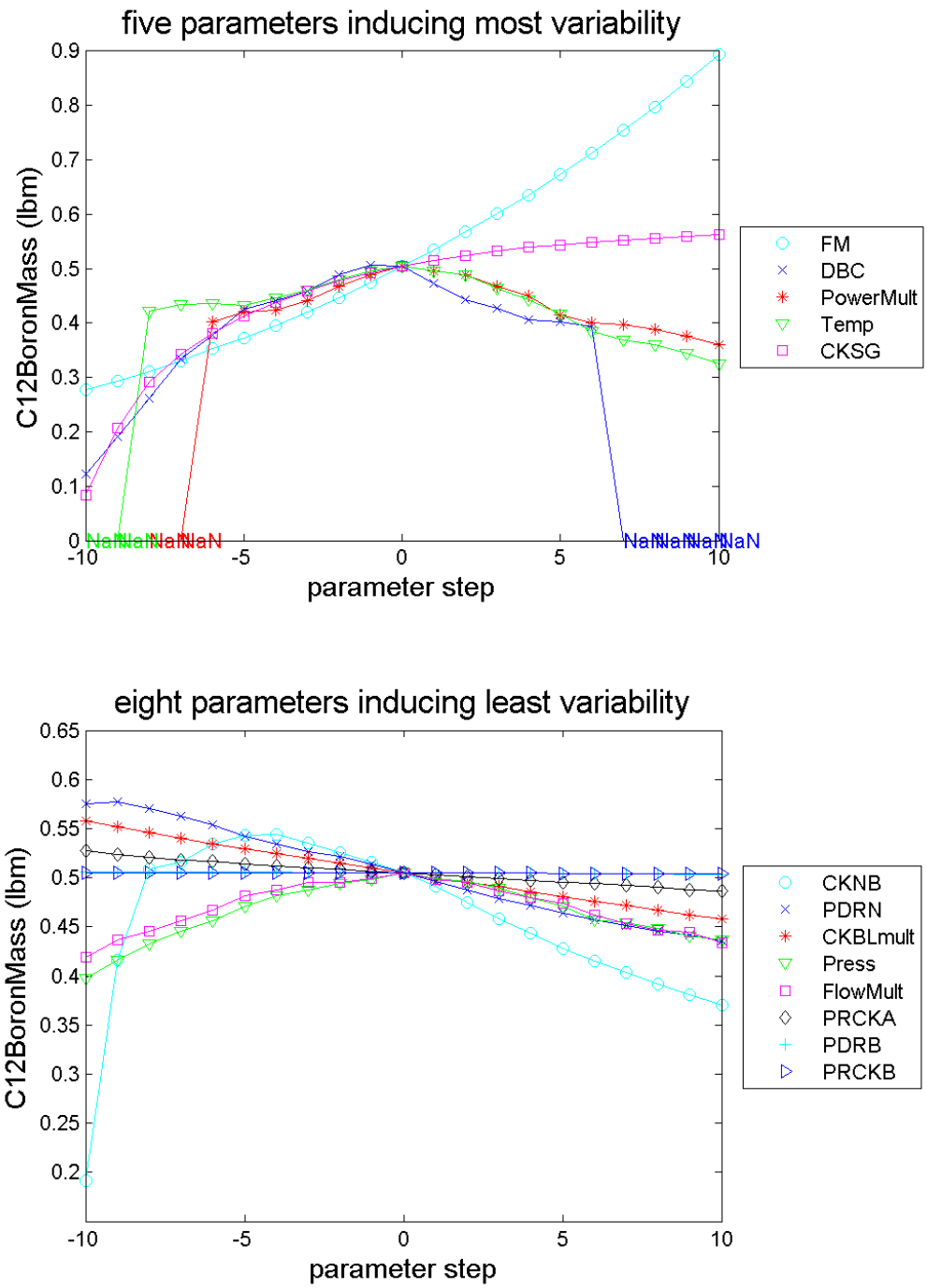

Figure 6. Univariate parameter sensitivities for end of cycle 12 boron mass (lbm).

Recommendations:

- Repeat this study, carefully examining the causes of individual simulation failures. Specifically, given issues with variations in power, temperature, and Dittus-Bolter correlation, verify that the VIPRE-W simulations are completing correctly.
- Investigate whether VIPRE-W and/or BOA are producing additional warnings not captured by the simulation infrastructure.
- Include corrosion product release factors (CRELNI and CRELFE, or alternately RFNI and RFFE as they are multiplied together) for these single-parameter studies, even though joint variation seems infeasible. If more sensitive, tt may be prudent to include these parameters, excluding others.

5.3. Global Sensitivity Analysis

The goal of global sensitivity analysis is to assess the influence of input parameters, considered jointly over their entire prescribed ranges, on the responses of interest. Figure 7 through Figure 13 show partial correlation coefficients calculated from the 1300 Monte Carlo samples (modulo any omitted failed samples). Each figure corresponds to one response metric of interest and shows the influence of each of the thirteen parameters, with separate bars for each cycle. Typically correlations with absolute values greater than 0.7 are considered highly significant, but given the samples sizes in this study, all those greater than 0.2 might be important for further consideration. (Note that some values are negligible and do not display on the plot.) From these, observe:

- overall the parameters PRCKB, PDRN, PDRB, CKNB, CKBLmult, and CKSG have comparably little influence on any of the responses (though there are some exceptions);
- DBC has strong effect on most of the responses, but particularly on the nickel/iron ratio, quantities of nickel and iron, and crud thickness;
- FM primarily influences boron mass, and to a lesser extent crud thickness;
- PRCKA strongly influences nickel metal mass, and therefore the nickel/iron ratio;
- the thermal-hydraulic parameters most influence the nickel and iron concentrations; and
- perhaps surprisingly the same parameter has a positive correlation in some cycles, but negative in other cycles, e.g., DBC shown in Figure 7. This warrants further investigation.

Figure 14 shows scatter plots of all seven responses vs. the three most influential BOA parameters. These highlight the strong correlation of DBC with all responses and FM especially with boron mass. From the plot of CKNB versus CrudFraction observe that correlation coefficients can be misleading as in this case, there appears to be a nonlinear relationship between the input and output.

This sensitivity analysis is a crucial precursor to planned work to calibrate BOA to plant measurement data. The BOA parameter estimation process should focus primarily on the parameters revealed most sensitive by this study and secondarily on those with less influence.

Recommendations:

- Include the likely highly sensitive parameters RNFI and RFFE (or CRELNI, CRELFE, respectively) in a follow-on study.
- Use Sobol indices or higher-order regression to assess whether there are significant nonlinear or interaction affects between multiple parameters and responses. Investigate the sensitivity of parameters whose sense changes from cycle to cycle.
- Assess whether there are observational data available to inform the most sensitive parameters and possibly further constrain their ranges. For example, a previous preliminary calibration study [3] suggests that even coarse crud index data supports a reduced range for DBC. Explicitly leveraging the spatial component of data as was done in that study, instead of the integral quantities of the present study, should help further refine these estimates. In addition to using crud index data, future studies should explore chemistry, composition, and thickness data if available, in coordination with both industry partners and the CASL validation data program.

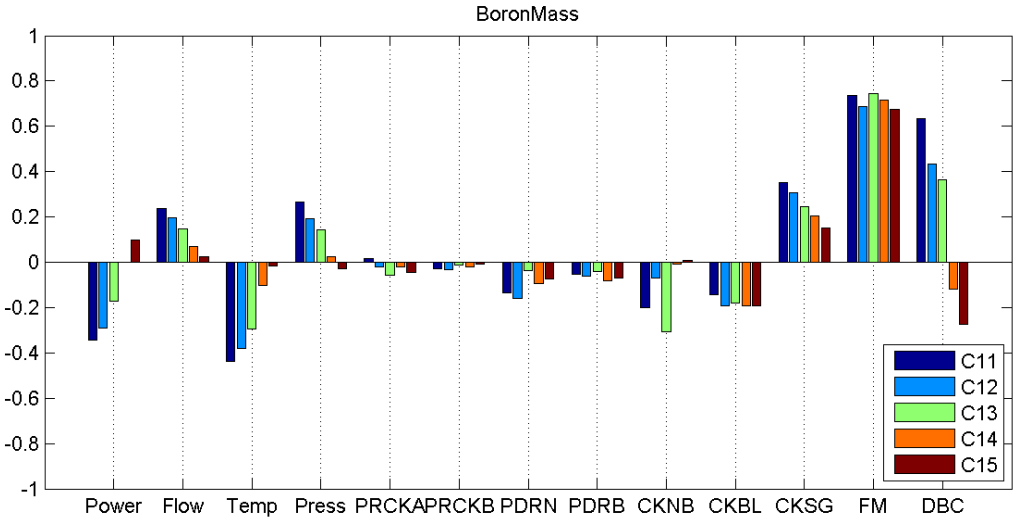

Figure 7. Partial correlation of BoronMass with each input.

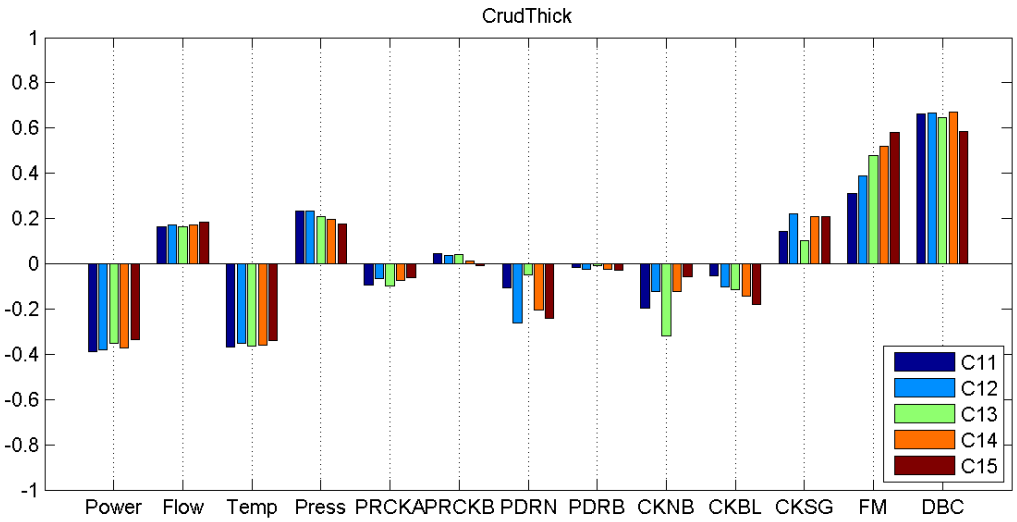

Figure 8. Partial correlation of CrudThick with each input.

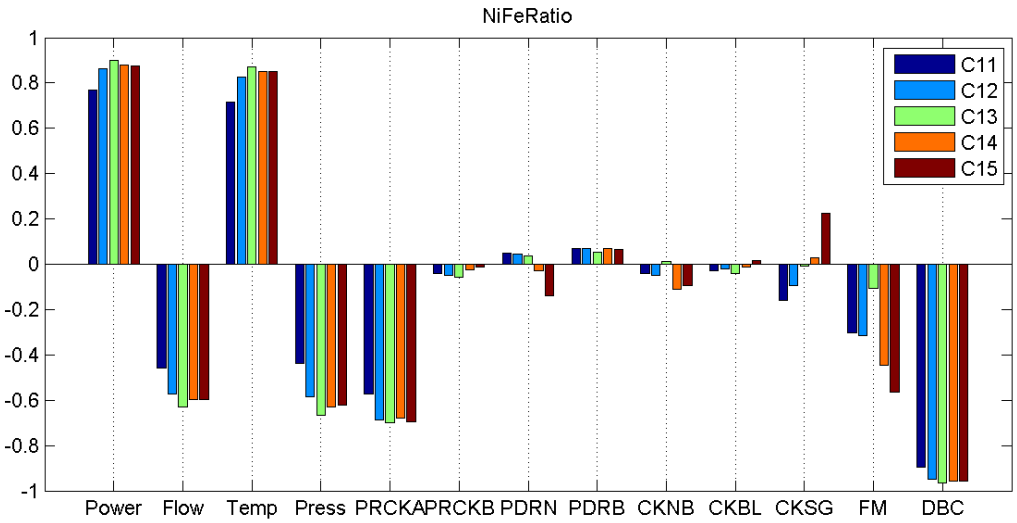

Figure 9. Partial correlation of NiFeRatio with each input.

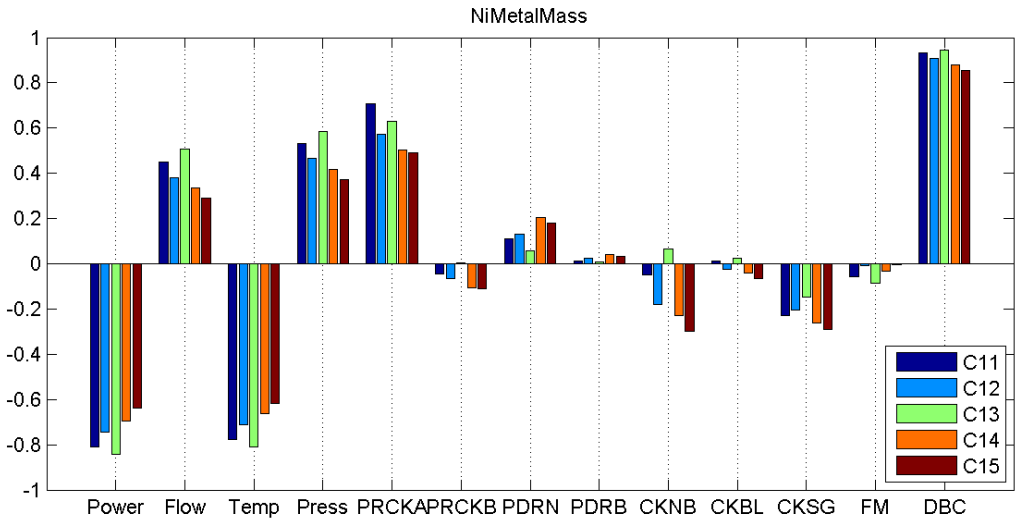

Figure 10. Partial correlation of NiMetalMass with each input.

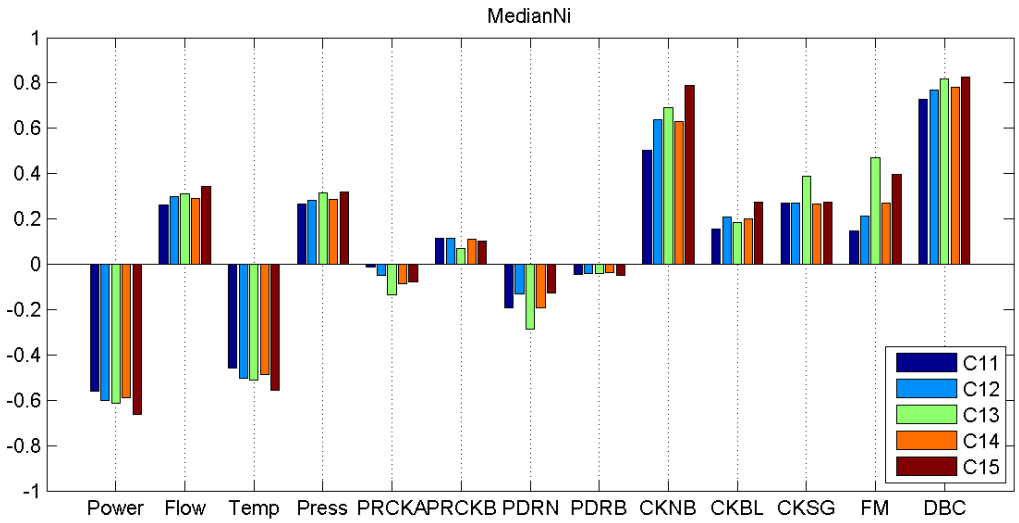

Figure 11. Partial correlation of MedianNi with each input.

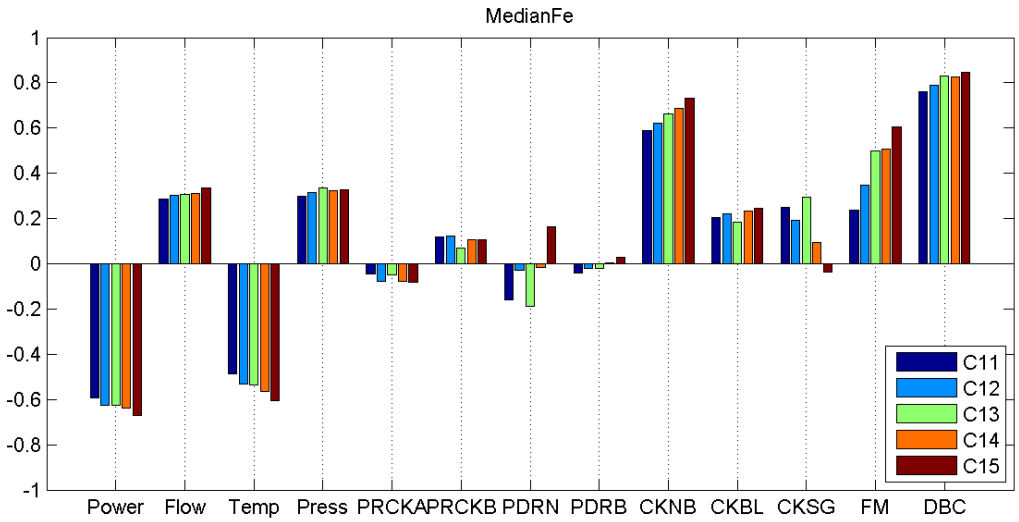

Figure 12. Partial correlation of MedianFe with each input.

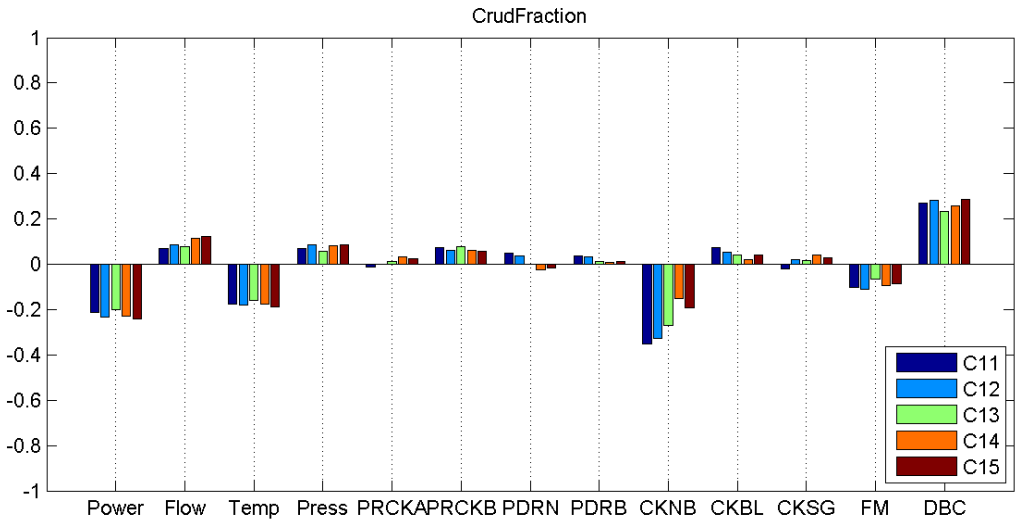

Figure 13. Partial correlation of CrudFraction with each input.

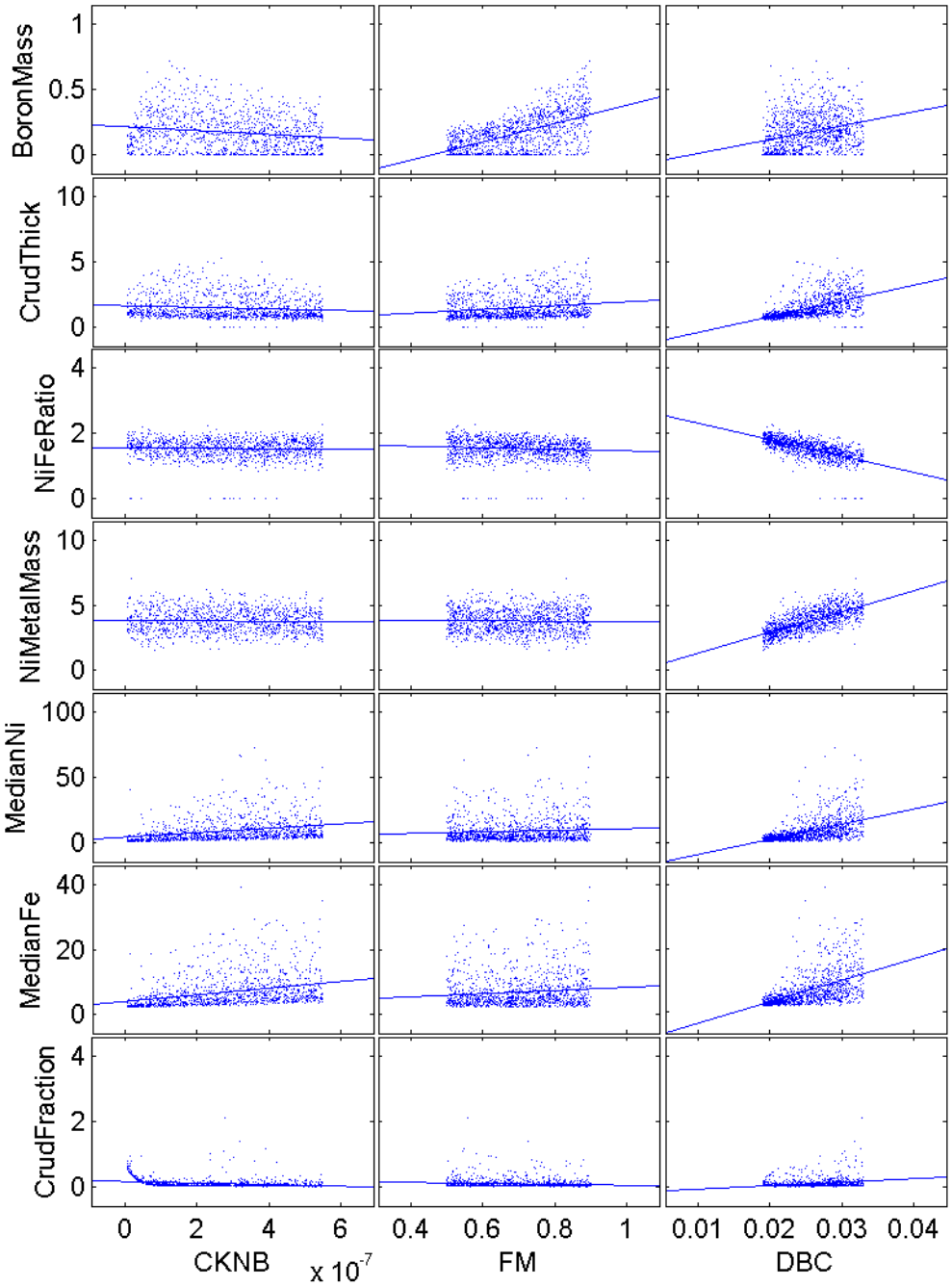

Figure 14. Response scatter plots and regression lines for most influential BOA parameters.

5.4. Global Uncertainty Quantification

The goal of global uncertainty propagation is to compute statistics in output response metrics based on available information about the uncertainty of input parameters. Such studies are strongly dependent on the assumed prior uncertainty distributions.

DAKOTA's summary statistics, based on 1300 samples attempted (failed results noted above) are shown in Table 11, along with a calculated coefficient of variation. For comparison, statistics using a third-order polynomial chaos expansion (PCE, via regression on the pre-computed LHS samples) are also shown. Figure 15 through Figure 21 use histogram plots to illustrate the overall range of variation realized in the seven responses. Throughout this section, units are as in Table 2. From these we note:

- The largest overall relative variability, as indicated by coefficient of variation, is in CrudFraction, the EOC to BOC ratio of core crud mass, and it increases with cycle (though the absolute values do not).
- Figure 21 indicates numerous outliers for the CrudFraction response, which affect the coefficient of variation. When removed, the coefficient of variation for this response is significantly reduced and more consistent across cycles: 1.59, 1.86, 1.74, 1.47, and 1.99 for cycles 1 through 5, respectively (though these are still large variations). Further investigation into the cause of the outliers is warranted.
- Significant variability is also observed in boron mass, median nickel, and crud thickness, with median iron following.
- The output distributions are all unimodal, though there are clear differences in range and shape of variability across cycles 11—15.

Recommendations:

- Resolve simulation failures to be able to apply failure-sensitive PCE approaches based on fixed quadrature points.
- Conduct a convergence study with more samples to verify that statistics have converged and assess reliability of potentially more efficient stochastic expansion-based methods for this problem. *This is already underway.*
- Discuss with industry the predicted ranges of uncertainty, not just in terms of ranking, but overall range of variability and potential impact on CIPS determinations. In particular determine parameter regimes with high probability of inducing responses above critical thresholds.

Table 11. Response statistics from 1300 Monte Carlo samples.

response		stats from samples			stats from PCE		
		mean	std dev	coeff var	mean	std dev	coeff var
Cycle 11	BoronMass (lbm)	0.170	0.141	0.83	0.167	0.153	0.92
	CrudThick (mils)	1.453	0.866	0.60	1.582	0.994	0.63
	NiFeRatio (1)	1.524	0.298	0.20	1.439	0.380	0.26
	NiMetalMass (lbm)	3.798	0.908	0.24	3.987	1.036	0.26
	MedianNi (ppb)	8.738	8.950	1.02	10.752	11.471	1.07
	MedianFe (ppb)	6.810	5.033	0.74	7.981	6.387	0.80
	CrudFraction (1)	0.087	0.148	1.71	0.120	0.182	1.52
Cycle 12	BoronMass (lbm)	0.342	0.215	0.63	0.332	0.239	0.72
	CrudThick (mils)	1.872	1.250	0.67	2.205	1.560	0.71
	NiFeRatio (1)	1.725	0.349	0.20	1.537	0.487	0.32
	NiMetalMass (lbm)	6.915	1.696	0.25	7.619	2.067	0.27
	MedianNi (ppb)	7.078	5.543	0.78	9.645	8.050	0.83
	MedianFe (ppb)	5.043	2.805	0.56	6.408	4.052	0.63
	CrudFraction (1)	0.100	0.234	2.33	0.187	0.311	1.66
Cycle 13	BoronMass (lbm)	0.144	0.166	1.15	0.151	0.175	1.16
	CrudThick (mils)	1.303	0.716	0.55	1.514	0.920	0.61
	NiFeRatio (1)	1.662	0.407	0.24	1.444	0.560	0.39
	NiMetalMass (lbm)	1.619	0.441	0.27	1.838	0.577	0.31
	MedianNi (ppb)	10.116	7.012	0.69	12.599	9.134	0.72
	MedianFe (ppb)	7.736	4.567	0.59	9.569	5.899	0.62
	CrudFraction (1)	0.076	0.179	2.34	0.139	0.235	1.68
Cycle 14	BoronMass (lbm)	0.382	0.279	0.73	0.327	0.336	1.03
	CrudThick (mils)	2.095	1.247	0.60	2.326	1.464	0.63
	NiFeRatio (1)	1.941	0.528	0.27	1.670	0.709	0.42
	NiMetalMass (lbm)	6.970	1.695	0.24	7.563	2.088	0.28
	MedianNi (ppb)	8.959	7.452	0.83	12.637	10.769	0.85
	MedianFe (ppb)	5.084	2.700	0.53	6.539	3.806	0.58
	CrudFraction (1)	0.165	0.636	3.84	0.368	0.829	2.25
Cycle 15	BoronMass (lbm)	0.342	0.270	0.79	0.277	0.337	1.22
	CrudThick (mils)	1.897	0.954	0.50	1.938	1.146	0.59
	NiFeRatio (1)	2.237	0.596	0.27	1.934	0.800	0.41
	NiMetalMass (lbm)	6.140	1.469	0.24	6.568	1.735	0.26
	MedianNi (ppb)	6.487	4.224	0.65	8.545	5.624	0.66
	MedianFe (ppb)	4.090	1.613	0.39	4.880	2.106	0.43
	CrudFraction (1)	0.109	0.432	3.96	0.244	0.571	2.34

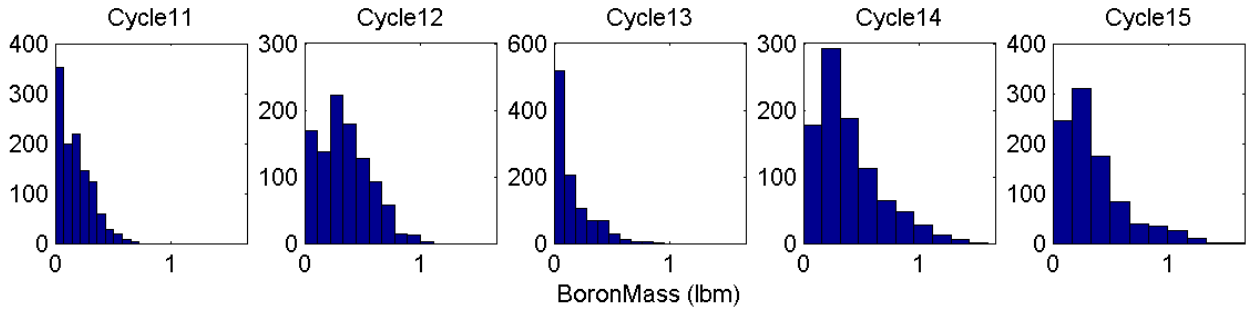

Figure 15. BoronMass uncertainty (histogram) for each cycle.

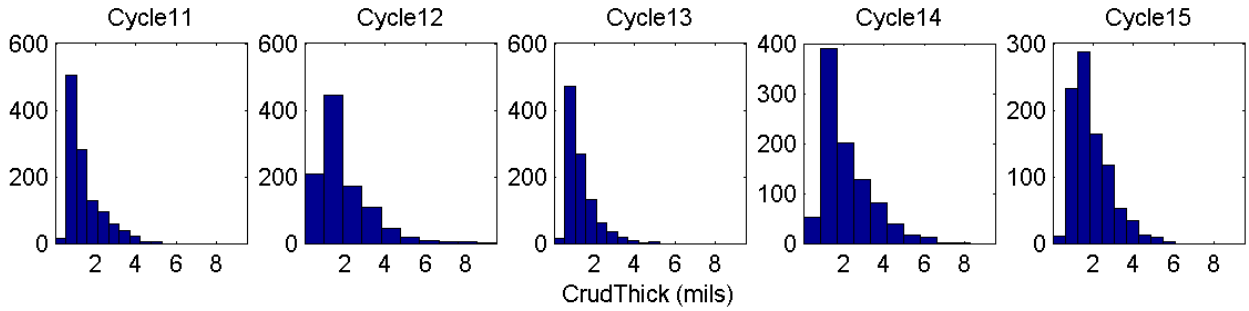

Figure 16. CrudThick uncertainty (histogram) for each cycle

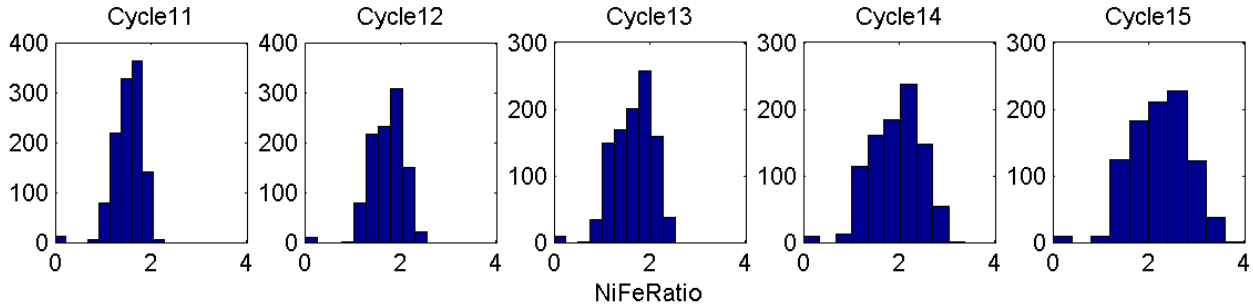

Figure 17. NiFeRatio uncertainty (histogram) for each cycle.

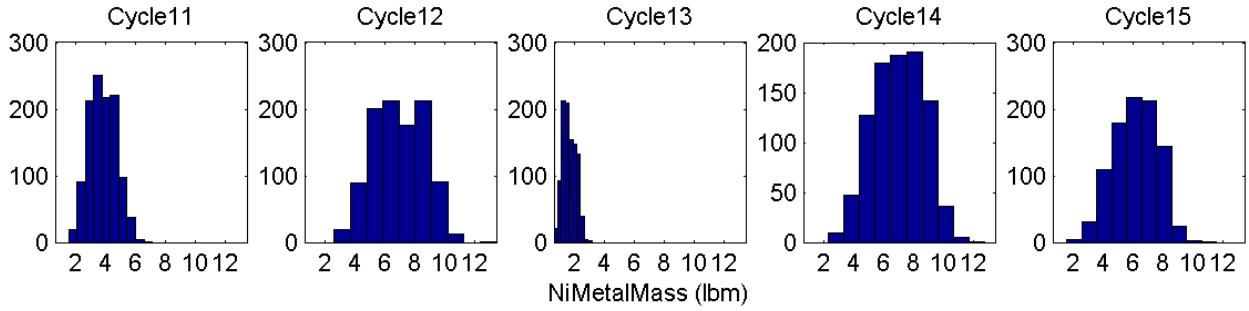

Figure 18. NiMetalMass uncertainty (histogram) for each cycle.

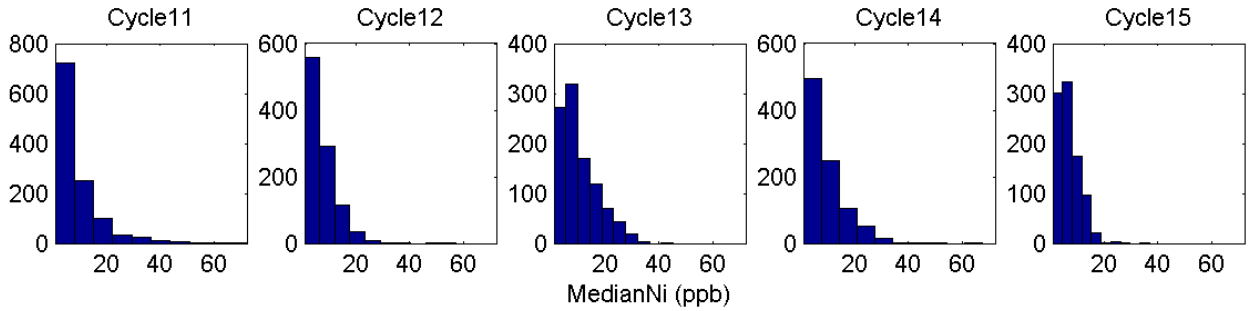

Figure 19. MedianNi uncertainty (histogram) for each cycle.

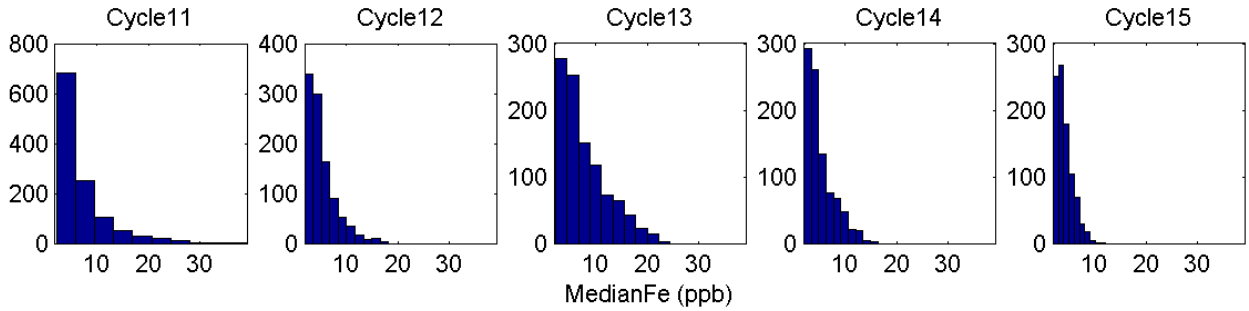

Figure 20. MedianFe uncertainty (histogram) for each cycle.

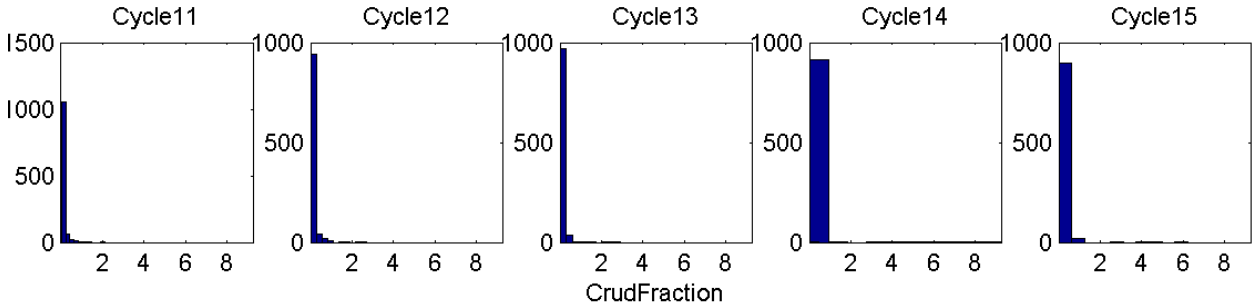

Figure 21. CrudFraction uncertainty (histogram) for each cycle.

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6. SUMMARY AND FUTURE WORK

This VUQ-led Level 1 milestone demonstrated DAKOTA-based statistical sensitivity and uncertainty quantification with coupled VIPRE-W and BOA codes. In extending previous studies [2, 3] on crucial PWR problems, it investigated two-coupled physics and response metrics more directly predictive of CIPS, with the goal of assisting the industry in determining the most crucial factors and associated uncertainties. To our knowledge, this is the most extensive statistical study to date exercising coupled VIPRE-W (or VIPRE-01)/BOA tools in joint parametric variation. It identified a number of important challenges with respect to characterization of multivariate uncertainties, code robustness, and leveraging domain knowledge to guide the VUQ process.

The studies provide a better understanding of the CASL CIPS challenge problem as well as strengths and limitations of the current predictive tool. Near-term investigations are needed to do the following, prior to any follow-on advanced studies:

- Carefully investigate the robustness of the workflow and simulation tools (given observed "failure" with modest single parameter variations) and the validity of the attempted joint parameter variations, including for omitted parameters.
- Investigate potential effects of corrosion product release factors, as these are believed by industry to be crucial (and caused simulation failure in the present computational studies). If CASL's MAMBA tool will only address boron holdup and crud deposition models, relying on BOA's crud source models, it will be crucial to characterize the source terms using field data (e.g., coolant chemistry data), or otherwise adjust models to reduce their sensitivity. This might mean CASL has to better understand some out-of-core phenomena like crud sources to make better in-core predictions.
- Assess convergence of statistics in the uncertainty quantification methods and discuss results with industry to understand potential impact on CIPS determinations.

This work lays an important foundation for follow-on studies with more sophisticated coupled physics and advanced simulation models. A notable limitation of the present study is lack of coupling to a neutronics analysis package, which could significantly change the results of this study, given the effects of boron and other crud products on heat flux and consequently, boiling. This will be addressed in an upcoming 2012 CASL VUQ milestone, as will migration to next-generation analysis tools for neutronics, thermal-hydraulics, and crud. Also upcoming will be data-driven calibration and validation studies to hopefully reduce uncertainty in the parameter characterizations and tighten bounds on predictions.

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