Uncertainty Quantification of EBR-II Loss of Heat Sink Simulations with SAS4A/SASSYS-1 and DAKOTA

G. Zhang¹, T. Sumner¹, T. Fanning¹

¹Argonne National Laboratory, Argonne, IL, USA

E-mail contact of main author: gzhang@anl.gov

Abstract. Argonne has developed SAS4A/SASSYS-1 models for the benchmark analyses of the Experimental Breeder Reactor II (EBR-II) Balance-of-Plant (BOP) tests that represented protected and unprotected loss of heat sink conditions. Some assumptions had to be made for the models because of uncertainties related to the cooling system. In addition, the reactivity feedback coefficients also have uncertainties due to the nuclear data. These uncertainties may contribute to discrepancies observed between the simulation results and the measured data. The objective of this study is to apply the recently developed coupling between Dakota and SAS4A/SASSYS-1 to investigate the impact of uncertainties on the simulation results. The sensitivity analysis helps determine the prioritization of future R&D efforts. Dakota is an uncertainty quantification and optimization toolkit. It was coupled with SAS4A/SASSYS-1 via a Python interface to meet an increased need to perform sensitivity analyses and uncertainty quantification in the advanced reactor domain. Dakota was used to sample userspecified parameters, drive SAS4A/SASSYS-1 transient simulations, and quantify statistical metrics as part of post processing. The studies described in this paper include the uncertainty quantification of the EBR-II simulations and calibration between the simulation results and the experimental data. By applying Dakota for uncertainty propagation, it is found that the radial expansion, control rod drive expansion, and stagnant sodium mixing models have significant impacts on the benchmark results. Following the uncertainty quantification, parameters in the EBR-II model that were identified to have significant impacts were optimized by Dakota in order to assess the magnitude of changes needed to improve the simulation results.

Key Words: EBR-II, Loss-of-Heat-Sink, Uncertainty Quantification, Calibration.

1. Introduction

Advancements in the knowledge of nuclear reactor performance have led to an increased need to perform Sensitivity Analyses (SA) and Uncertainty Quantification (UQ) in the advanced reactor domain. The role of uncertainty quantification spans many facets in the nuclear industry, including system design and optimization, licensing, and probabilistic risk assessment [1].

SAS4A/SASSYS-1 [2], which is developed by Argonne National Laboratory, is a system code for Sodium-cooled Fast Reactor (SFR) transient safety analysis. It has been recently coupled with Dakota via a Python interface to extend the capabilities of the Argonne safety code for uncertainty quantification and design optimization. The Dakota software [3], maintained by Sandia National Laboratory, is an uncertainty quantification and optimization toolkit that has been in development for over 20 years. With the new coupling package, Dakota samples user specified parameters, performs SAS4A/SASSYS-1 transient simulations with those parameters, and completes post processing by quantifying statistical metrics. Dakota is also capable of performing calibration in order to resolve discrepancies between the simulation results and the experimental data.

The objective of this study is to use the recently coupled Dakota-SAS4A/SASSYS-1 package to evaluate the impact of uncertainties on EBR-II SAS4A/SASSYS-1 simulations. Such kinds of sensitivity analyses help determine the prioritization of future R&D efforts. Two EBR-II Balance-of-Plant (BOP) benchmark cases were repeated with the parameters recommended by Dakota and the agreement between the SAS4A/SASSYS-1 results and the measured data was improved significantly.

2. EBR-II SAS4A/SASSYS-1 Model

Argonne developed EBR-II SAS4A/SASSYS-1 models for the benchmark analysis of two loss-of-heat-sink tests, BOP-301 and BOP-302R [4]. These two tests were conducted to demonstrate the capability of passive reactor shutdown and decay heat removal in response to unprotected transients. This analysis was performed as part of knowledge preservation activities in support of validation of simulation tools and models in the area of SFR development. Comparisons with experimental data and other safety codes provide the opportunities to improve SFR computational codes and methods.

The BOP tests were conducted during the Shutdown Heat Removal Test (SHRT) program. During the BOP tests, the intermediate sodium pump tripped without scramming the control rods or tripping the primary pumps. One such test, BOP-301, began at half power and was performed five days before SHRT-45R. A similar test, BOP-302, was performed the following day starting from full power. Four days later, several hours after SHRT-45R, BOP-302 was repeated as BOP-302R. These two BOP tests are of particular interest because the primary flow rates remained high enough that the uncertainty in the primary flowmeter readings was low. The initial conditions of these two BOP tests are shown in TABLE I [4].

Parameter	BOP-301	BOP-302
Power	31.0 MW	59.9 MW
Primary Mass Flow Rate (Core + Bypass)	472.6 kg/s	470.8 kg/s
Intermediate Mass Flow Rate	202.2 kg/s	307.2 kg/s
Core Inlet Temperature	616.9 K	616.4 K
Auxiliary EM Pump Head	100%	100%

TABLE I BOP-301 AND BOP-302R INITIAL CONDITIONS

Previous benchmark results of the two BOP tests were in good agreement with selected measured data. However, it was observed that the predicted inlet temperatures increased more rapidly than the measurements; the temperatures at the end of the BOP-301 simulation were 5K lower than the measured temperatures. For the BOP-302R case, the difference between the measurements and simulation temperatures was as much as 4K at the end of the test as well.

SAS4/SASSYS-1 simulations of the EBR-II BOP tests involve many uncertainties that may produce the observed discrepancies. As an example, the sodium cold pool in the model was initially split into two parts, as illustrated in FIG. 1 [4]. The horizontal dashed line is the boundary between the upper and lower sodium volumes. When the primary pumps trip, the lower part is usually assumed to be stagnant, and coolant mixing occurs slowly due to the large volume of the cold pool. However, since the primary pumps remain on during the BOP tests, coolant in the lower cold pool volume is continuously pumped to the core. As a result,

coolant mixing becomes much more important and significantly affects the simulation results. The coolant mixing can be represented in a very simplified form as

$$Q = \dot{m}c_p \Delta T$$

where \dot{m} is an assumed mixing flow rate, c_p is the sodium heat capacity, and ΔT is the temperature difference between the two pools.

The component-to-component heat transfer model was used to represent the flow mixing between the upper and lower cold pool volumes:

$$Q = hA\Delta T$$

where h is the heat transfer coefficient and A is the heat transfer surface area, both of which are assumed to be constant. By assuming that \dot{m} and c_p are constant, $h \times A$ can be set to $\dot{m} \times c_p$ to achieve a similar effect as the stagnant volume flow mixing model. This model is based on a stagnant volume flow mixing model developed for the SAM code and more details are available in Reference [5].

The volumes of sodium in the upper and lower cold pools along with the heat transfer coefficient used for this model were initially chosen based on engineering judgment. It should be noted that CFD analyses are required to properly understand the thermal stratification along the Z-Pipe, at the IHX inlet, and in the cold pool. SAS4A/SASSY-1 has been coupled with a CFD code and the thermal stratification will be investigated in the future.

The study in this paper evaluates the impacts of these assumptions on the benchmark results. Following the sensitivity analyses, the uncertain parameters that have relatively large impacts were optimized by Dakota to assess the magnitude of changes needed to improve the agreement between the simulation results and the measured data.



FIG. 1: PRIMAR-4 model for EBR-II primary system [4].

3. Dakota and SAS4A/SASSYS-1 Coupling

A Python interface was developed to couple Dakota with SAS4A/SASSYS-1. The Dakota executable is available pre-compiled via the Sandia National Laboratory website [3], and coupling with SAS4A/SASSYS-1 (or any software) is accomplished via a black-box interface. Data communication between Dakota and SAS4A/SASSYS-1 occurs through parameter and response files. Uncertain parameters in the SAS4A/SASSYS-1 input template are replaced with random values generated by Dakota. Then, SAS4A/SASSYS-1 simulations are initiated, and the response values of interest from the SAS4A/SASSYS-1 simulation are saved for processing by Dakota. FIG. 2 illustrates this coupling scheme.



FIG. 2: Dakota and SAS4A/SASSYS-1 coupling scheme.

A Dakota input file is composed of the methodology, variables, interface, and responses for the uncertainty quantification and design optimization process. A series of sampling-based techniques is implemented in Dakota for uncertainty propagation. The Monte Carlo method is one of the most popular sampling techniques and involves random sampling with specific distributions on the uncertain domain. Another sampling-based technique for uncertainty propagation, Latin Hypercube Sampling illustrated in FIG. 3, is used for the uncertainty quantification of the BOP simulations. The Latin Hypercube Sampling (LHS) is a method for exploring the input space of an uncertain domain divided into N segments. The relative length of each segment is determined by the probability distribution. Every subgroup in each of the uncertain variables is randomly assigned to a sample only one time. There is no restriction on the number of bins, but the LHS requires all uncertain variables to have the same number of bins. The total number of samples equals the number of bins. LHS is expected to require fewer samples than traditional Monte Carlo method to achieve the same statistical accuracy [3].

The responses of interest are written in a result file and returned to Dakota for the quantification of the statistical metrics. Means, standard deviations, and 95% confidence intervals are computed for each of the responses. In addition, Dakota calculates the most common statistics between uncertainties and responses of interest, such as the covariance, Pearson coefficient, simple, partial, and rank correlations. The Pearson coefficient is a measure of the linear correlation between two variables, and its value is in a range between +1 to -1, inclusive. A Pearson coefficient with a large absolute value means that two variables are strongly correlated. A positive Pearson coefficient stands for a positive correlation while a negative value indicates that the two variables are inversely correlated.



FIG. 3: Examples of Monte Carlo and Latin Hypercube Sampling techniques.

4. Sensitivity Analysis of the EBR-II BOP Simulation

The sensitivity analysis was conducted to evaluate the impacts of the uncertainties existing in the simulations of the BOP tests. The uncertainties considered in this study are in the following categories:

- Reactivity feedback coefficients
- Technical specifications of the IHX
- Flow conditions in the cooling systems (e.g. flow rates, flow resistance)
- Boundary conditions (e.g. the steam generator outlet temperature)
- Coolant mixing model in the cold pool

The space-dependent reactivity coefficients for each reaction (i.e. fuel, cladding, coolant, Doppler reactivity coefficients) were treated as correlated parameters such that they were perturbed by the same fraction. Fourteen uncertainties summarized in TABLE II were considered for the EBR-II model. The variables were assumed to be uniformly distributed within the ranges determined by engineering judgement.

SAS4A/SASSYS-1 supports a simple radial core expansion reactivity feedback model. It assumes that the grid plate expansion is proportional to either the core inlet sodium temperature or the temperature of the walls in the inlet plenum; expansion of the duct walls is assumed to be proportional to the average temperature change of the structure near the load pads. While EBR-II did not have load pads, each subassembly had pressed dimple-type spacer buttons on the outside of the subassembly near the core midplane. These spacer buttons were intended to prevent core compaction [4]. In the EBR-II SAS4A/SASSYS-1 model, the ratio of XMC to XAC was treated as a variable to account for the expansion at the location of the spacer buttons near the core midplane.

$$\Delta \rho_{radial} = C_{radial} [\Delta T_{inlet} + \frac{XMC}{XAC} (\Delta \overline{T}_{load \ pads} - \Delta T_{inlet}]$$

Where

 $\Delta \rho_{radial}$ = reactivity change due to radial core expansion, \$

 C_{radial} = radial expansion reactivity coefficient, \$/K

 ΔT_{inlet} = core inlet temperature change, K

XMC = distance from the grid plate to the core midplane, m

XAC = distance from the grid plate to the above core load pads, m

 $\Delta \overline{T}_{load \ pads}$ = average structure temperature change at the load pad elevation, K.

A selection of simulated results was compared against the measurements, including

- Z-pipe inlet temperature
- High- and low-pressure inlet plena (HPP, LPP) temperatures
- Normalized power

Since the experimental data and the SAS4A/SASSYS-1 simulation results were at different time intervals, the SAS4A/SASSYS-1 simulation results were processed by piecewise linear interpolation. Then, the Root Mean Square (RMS) between the simulation results and experimental data was calculated as a measure of the agreement. Therefore, a lower RMS value means that the SAS4A/SASSYS-1 simulation results are closer to the measurements.

The Latin Hypercube Sampling technique was applied for the uncertainty propagation, and the fourteen uncertain parameters were perturbed simultaneously within the user-specified range in TABLE II. The Pearson coefficient between the perturbed uncertainty and the RMS value is an indicator of the agreement between the benchmark results and the measured data. Since the fourteen variables are investigated simultaneously, it is computationally expensive to converge the results. Instead, each of the uncertainties is assigned a score based on a binned approach such that two uncertainties exhibit similar impacts if the calculated Pearson coefficients fall within the same bin range. "+" (IPearson Coefficientl > 0.05) means that the measured and simulated data get closer by perturbing the variable; "++" (IPearson Coefficientl < 0.05) means the perturbation of the uncertain variable has limited impacts on the simulation results.

TABLE II shows the impacts of the uncertain variables on the EBR-II BOP-301 simulation. During a loss of heat sink transient, the radial core expansion contributes the most negative reactivity feedback. The control rod driveline expansion also provides a large amount of negative reactivity. Therefore, the related parameters have significant impacts on the benchmark results. On the contrary, the axial expansion and Doppler reactivity feedback effects impose relatively small positive feedbacks for the BOP tests, and therefore their impacts are very limited.

Since the primary pumps remained on during the BOP tests, significant sodium mixing occurred between the upper and lower sodium volumes, and the corresponding parameters (i.e. lower sodium pool volume and heat exchange coefficient) strongly affect the simulation results. The perturbation of the initial primary flow rate affects the core outlet temperature (i.e. Z-pipe inlet temperature), and therefore improves the agreement. The steam generator outlet temperature and the flow resistance of the intermediate loop serve as the boundary conditions in the SAS4A/SASSYS-1 model, and their effects on the primary loop are negligible. Sensitivity analysis also shows that the product of density and specific heat for the IHX tubes have a negligible impact on the benchmark results.

	Nominal Value	Range (Uniform Distribution)	Tz-pipe inlet	T _{HPP-} inlet	T _{LPP-} inlet	Power
Radial expansion feedback coefficient (\$/K)	-0.00266	±20%	++	++	++	+
XMC/XAC ratio	0.96546	0.0001 - 0.9999	++	++	++	++
Flooded Doppler coefficient $(\Delta k/k)$	space dependent	±20%	N/A	N/A	N/A	N/A
Fuel expansion coefficient $(\Delta k/k-kg)$	space dependent	±20%	N/A	N/A	N/A	N/A
Cladding expansion coefficient (Δk/k-kg)	space dependent	±20%	N/A	N/A	N/A	N/A
Coolant reactivity coefficient (Δk/k-kg)	space dependent	±20%	N/A	N/A	N/A	N/A
Control rod drive thermal expansion coefficient (1/K)	2.0×10 ⁻⁵	±30%	++	+	+	+
Control rod expansion feedback coefficient (\$/m)	-15.61	±20%	+	+	+	N/A
Heat exchange coefficient between upper and lower	298609	0.1 - 400000	++	++	++	N/A
Lower sodium pool volume (m ³)	186.576	40 - 260	++	++	++	++
Steam generator outlet temperature (K)	548	±10	N/A	N/A	N/A	N/A
Resistance in the intermediate loop	4000000	0.0 - 5000000.0	N/A	N/A	N/A	N/A
Initial primary flow rate (kg/s)	468.7	±5%	++	+	+	N/A
Density*specific heat of tube in IHX (J/m ³ -K)	4.36×10^{6}	±10%	N/A	N/A	N/A	N/A

TABLE II: IMPACTS OF UNCERTAIN VARIABLES ON EBR-II BOP-301 BENCHMARK RESULTS.

5. Optimization of EBR-II BOP Simulation Results

The sensitivity analysis described above demonstrates that the radial expansion, control rod drive expansion, and sodium pool mixing models have the largest impacts on the benchmark results. The Dakota-SAS4A/SASSYS-1 toolkit was used to identify the values for those input parameters such that the SAS4A/SASSYS-1 simulation results are in better agreement with the measured data for both BOP-301 and BOP-302R. The hybrid optimization method implemented in Dakota was used to find the global optima, and the input variables perturbed by Dakota are:

- Radial expansion reactivity feedback coefficient
- XMC/XAC ratio
- Heat transfer coefficient between upper and lower cold pool volumes
- Volume of sodium in lower cold pool
- Control rod drive thermal expansion coefficient
- Initial primary flow rate

Since the BOP-301 and BOP-302R cases were performed during the same testing window and had the same core load configuration, the optimized cases are expected to have similar radial expansion feedback coefficients and control rod drive thermal expansion coefficients. BOP-302R was initiated at a higher power level than BOP-301, and therefore the different structure temperatures result in a different distribution of the force on the space buttons. Because of this, different radial growths (i.e. XMC/XAC ratios) were searched for the BOP-302R and BOP-301 cases. Considering the large volume of the sodium pool and the fact that the flow rates in the two cases are close, the mixing model is assumed to be same. Therefore, the same heat transfer coefficient and lower pool volume were applied for both cases. The individual initial flow rate was searched for each case in order to accommodate the uncertainty of the primary flow rate. It should be noted that these assumptions are made only for demonstration purposes, and future SAS4A/SASSYS-1 analyses for the EBR-II BOP tests are required to verify these parameters.

The Dakota-SAS4A/SASSYS-1 coupling is capable of evaluating the objective responses from a multi-model study. In each sample, Dakota updates the BOP-301 and BOP-302R SAS4A/SASSYS-1 input files with the random values and the simulations are conducted independently. Four responses of interest in each BOP case are sent back to Dakota for post-processing, including

- Z-Pipe inlet temperature
- HPP inlet temperature
- LPP inlet temperature
- Normalized power

The RMS values are calculated between the simulation results and the experimental measurements. Dakota uses the optimization mode to minimize these RMS values. It initialized 350 samples on the whole uncertain domain shown in TABLE II and the global optimum was narrowed down to a small region. Then, Dakota continued the local search until the uncertain parameters converged to the optimized parameters given in TABLE III. FIG. 4-7 illustrate that the agreement between the SAS4A/SASSYS-1 predictions and the measurements are greatly improved.

According to TABLE III, the optimization changes are relatively modest, except the XMC/XAC ratio for the BOP-302R case. A less negative radial expansion coefficient suggested by Dakota is still within the uncertain range determined by engineering judgement. A much smaller XMC/XAC ratio in the BOP-302R case indicates that the inlet coolant temperature has a larger impact on the radial expansion model than the average structure temperature at the level of above core load pad. The different optimized XMC/XAC ratios are attributed to the different initial power levels, which affect the distribution of the force on space buttons. The heat transfer coefficient and the lower sodium pool volume are reduced by 32% and 41% of the corresponding reference values, respectively. These observations need to be verified by the future CFD analysis of the sodium pool.



FIG. 4: BOP-301 core and Z-Pipe inlet temperatures – original (a) vs. optimized (b) models.



FIG. 5: BOP-302R core and Z-Pipe inlet temperatures – original (a) vs. optimized (b) models.



FIG. 6: BOP-301 total power



FIG. 7: BOP-302R total power.

	Reference	BOP-301 Optimized	BOP-302R Optimized
Radial expansion feedback coefficient (\$/K)	-0.00266	-0.00222	-0.00222
Initial primary flow rate (kg/s)	468.7 for BOP-301 466.9 for BOP-302R	463.6	458.1
XMC/XAC ratio	96.5%	99.8%	29.7%
Heat transfer coefficient between upper and lower sodium pool (W/K)	298609	202208	202208
Lower sodium pool volume (m ³)	186.6	109.9	109.9
Control rod drive thermal expansion coefficient (1/K)	2.00×10 ⁻⁵	1.70×10 ⁻⁵	1.70×10 ⁻⁵

TABLE III: OPTIMIZED SAS4A/SASSYS-1 INPUTS FOR BOP-301 AND BOP-302R BENCHMARK

6. Summary and Conclusion

In order to address discrepancies observed between SAS4A/SASSYS-1 simulation results and experimental data, the Dakota-SAS4A/SASSYS-1 package was applied to quantitatively evaluate the assumptions used in the BOP simulations. Fourteen uncertainties were simultaneously perturbed within the specified ranges by the Latin Hypercube Sampling technique. Sensitivity analysis shows that the radial expansion, control rod drive expansion, and stagnant sodium mixing models have the largest impacts on the simulation results. This sensitivity analysis helps determine the prioritization of the future R&D efforts.

Following the uncertainty quantification, the input parameters identified to have large impacts on both BOP-301 and BOP-302R simulations were optimized by Dakota such that the SAS4A/SASSYS-1 simulation results are in better agreement with the measurements. It appears that the optimization changes are relatively modest. The recommended radial expansion coefficient is less negative but within the uncertain range from engineering judgement. The two optimized BOP simulations exhibit quite different radial growth (i.e. XMC/XAC ratio), and this is partially attributed to the different initial power levels. The lower sodium pool volume and the heat transfer coefficient are recommended with the smaller values by Dakota, and these need to be verified by the future CFD analysis.

Acknowledgements

Argonne National Laboratory's work was supported by the U.S. Department of Energy, Assistant Secretary for Nuclear Energy, Office of Nuclear Energy, under contract DE-AC02-06CH11357.

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