Quantifying Time-Dependent Uncertainty in the BEAVRS Benchmark using Time Series Analysis

by

Shikhar Kumar

B.S. Operations Research: Financial Engineering,
Columbia University (2015)

Submitted to the Department of Nuclear Science and Engineering
in partial fulfillment of the requirements for the degree of
Master of Science in Nuclear Science and Engineering

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

February 2018

© Massachusetts Institute of Technology 2018. All rights reserved.

Author .................................................................
Department of Nuclear Science and Engineering
January 23, 2018

Certified by ..........................................................
Benoit Forget
Associate Professor of Nuclear Science and Engineering
Thesis Supervisor

Certified by ..........................................................
Kord Smith
KEPCO Professor of the Practice of Nuclear Science and Engineering
Thesis Supervisor

Accepted by .........................................................
Ju Li
Battelle Energy Alliance Professor of Nuclear Science and Engineering
Professor of Materials Science and Engineering
Chair, Committee on Graduate Students
Quantifying Time-Dependent Uncertainty in the BEAVRS Benchmark using Time Series Analysis

by

Shikhar Kumar

Submitted to the Department of Nuclear Science and Engineering on January 23, 2018, in partial fulfillment of the requirements for the degree of Master of Science in Nuclear Science and Engineering

Abstract

Advances in computational capabilities have enabled the development of high-fidelity methods for large-scale modeling of nuclear reactors. However, such techniques require proper benchmarking and validation to ensure correct and consistent modeling of real problems. Thus, the BEAVRS benchmark was developed to legitimize the advancements of new 3-D full-core algorithms in the field of reactor physics. However, in order to address the issue of BEAVRS uncertainty quantification (UQ) of Uranium-235 fission reaction rate data, this thesis proposes a new method for measuring uncertainty that goes beyond merely conducting statistical analysis of multiple measurements at one given point in time. Instead, this work hinges on principles of time series analysis and develops a rigorous method for quantifying the uncertainty in using “tilt-corrected” data in an attempt to evaluate time-dependent uncertainty. Such efforts show consistent results across the four different methods and will ultimately assist in demonstrating that BEAVRS is a non-proprietary international benchmark for the validation of high-fidelity tools.

Thesis Supervisor: Benoit Forget
Title: Associate Professor of Nuclear Science and Engineering

Thesis Supervisor: Kord Smith
Title: KEPCO Professor of the Practice of Nuclear Science and Engineering
Acknowledgments

This work was supported through a grant from the U.S. Department of Energy Office of Nuclear Energy’s Nuclear Energy University Program (NEUP). This research made heavy use of the CASMO-5/SIMULATE-3 analysis tools, which were made available through Studsvik Scandpower, Inc.

First and foremost, I would like to thank my thesis co-supervisors Professors Benoit Forget and Kord Smith for launching me into the research field of nuclear reactor physics and continually pushing me to strive for the deepest level of understanding in any direction my findings take me. I am also extremely fortunate to have had Professor Koroush Shrivan selflessly guide me through this work and answer to my beck and call for even the simplest of problems. Additionally, I am incredibly thankful to Dr. Jingang Liang and Geoffrey Gunow for helping me get started with work related to BEAVRS uncertainty quantification.

My time at MIT has been a truly gratifying experience, and this is in no small part due to the immense amount of help and guidance I receive from my friends. I am very thankful to Lisa Magnano-Bleehan for her commitment to her work and to improving the quality of lives of students at MIT. I am enormously indebted to my roommates Guillaume Giudicelli, Stephen Tsz Tang Lam, and Kitty Perry, who have been tremendous role models and have kept propelling me forward especially during the toughest times of graduate school. I would also like to acknowledge Caitlin Fedio, Vanshil Shah, and Naimun Siraj for their continued friendship since college.

Finally, I am exceptionally grateful to my parents, Mukta Singh and Parag Kumar, who have supported me through my academic journey each step of the way with tremendous encouragement and unflagging love.
Contents

1 Introduction and Background
   1.1 The BEAVRS Benchmark ............................................. 11
      1.1.1 Benchmark Specifications .......................... 12
      1.1.2 Operating Data ............................................. 12
   1.2 Uses of the BEAVRS Benchmark ................................. 19
   1.3 Motivation for Uncertainty Quantification ..................... 22
   1.4 Model Specifications Using CASMO/SIMULATE ................. 24
   1.5 Outline for Thesis .............................................. 25

2 Uncertainty in Processing and Post-Processing of BEAVRS Data 26
   2.1 Extracting Detector Signals and Processing Data .............. 26
   2.2 Uncertainty Quantification through Theoretical Analysis of Axial Un-
      certainties .................................................. 28
      2.2.1 Uncertainty from Measurement .......................... 28
      2.2.2 Uncertainty from Interpolation ......................... 31
      2.2.3 Uncertainty from Axial Realignment .................... 32
      2.2.4 Uncertainty from Spline Fitting ......................... 34
      2.2.5 Uncertainty of Axially Integrated Radial Data ......... 34
   2.3 Uncertainty Quantification through Multiple Measurements .... 35
   2.4 Motivation for Time Series Analysis ........................... 36

3 Uncertainty in Using Tilt-Corrected BEAVRS Data 38
   3.1 Generation of Tilt-Corrected Data ............................... 39
   3.2 Initial Gap Test to Mimic Tilt in BEAVRS Data ............... 41
   3.3 Methodology for Tilt-Correction Uncertainty Quantification 43
   3.4 Evaluation of Tilt-Correction Uncertainty .................... 50
   3.5 Interpretation of Results .................................... 52

4 Time Dependent Uncertainty in the BEAVRS Benchmark Using
       the CASMO/SIMULATE Model ...................................... 54
   4.1 Visualization of Core-wide RMS .................................. 56
   4.2 Characterization of Model Bias .................................. 57
   4.3 Quantifying Detection Uncertainty Over Entire Burnup Range ... 60
   4.4 Validation of Assumptions for the CASMO/SIMULATE Model .... 62
   4.5 Verification of Results with Other Simulation Tools .......... 66
List of Figures

1-1 Cycle 1 core enrichment zones and burnable absorber positions . . . . 13
1-2 Cycle 2 shuffling pattern and burnable absorber positions . . . . . . . 14
1-3 Cycle 1 detailed burnable absorber view . . . . . . . . . . . . . . . . 15
1-4 Core cross-section . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 16
1-5 Scale view of all axial planes. . . . . . . . . . . . . . . . . . . . . . . 17
1-6 Instrument tube positions. . . . . . . . . . . . . . . . . . . . . . . . . 18
1-7 Initial raw detector measurements (top to bottom) [1]. . . . . . . . . 19
1-8 Detector measurements with gain factors applied (top to bottom) [1]. 19
1-9 Detector measurements with zero points removed (top to bottom) [1]. 20
1-10 Detector measurements within assembly J10 (top to bottom) [1]. . . 20
1-11 All detector signals before realignment [1]. . . . . . . . . . . . . . . . 21
1-12 All detector signals after realignment [1]. . . . . . . . . . . . . . . . 21
1-13 Comparison of all assemblies after spline [1]. . . . . . . . . . . . . . . 22
1-14 Final processed HZP measurement data [1]. . . . . . . . . . . . . . . 22
1-15 Radial detector measurements at HZP (axially integrated) [1]. . . . 23

2-1 Ranges and distributions of four types of measured data in cycle 1 [2]. 29
2-2 Multiple measurements example. Assembly H11 was measured twice
by Detector 3. The average and relative sample standard deviation
(RSTD) is calculated for every axial measurement point [2]. . . . . . . 30
2-3 Axial signal uncertainty from all multiple measurements in cycle 1.
Top: A plot of the average and relative sample standard deviation
of all multiple measured data points. Bottom: A plot that divides the
data points into groups and calculates the 95\% confidence values for all
groups to represent as a measurement uncertainty table [2]. While the
overall distribution is not normally distributed, statistics within each
group follows a normal distribution. . . . . . . . . . . . . . . . . . . . . . 32
2-4 A representation of axial interpolation uncertainty. Top: Interpolation
errors along with axial locations. Bottom: Interpolation uncertainty
table using 95\% confidence values for all locations [2]. . . . . . . . . 33
2-5 A representation of axial extrapolation uncertainty. Top: Distribution
of extrapolation errors for 6 axial locations. Bottom: Extrapolation
uncertainty table using 95\% confidence values for all locations [2]. . . 34
2-6 Radial assembly measurements with uncertainties calculated from axial
uncertainties at HZP in Cycle 1. The top number is normalized assembly
signal while the bottom number is its uncertainty [2]. . . . . . . . . . . 36
2-7 Distribution of radial data uncertainty calculated from axial uncertainties in cycle 1 [2].

3-1 Radial detector measurements at HZP (axially integrated) [1].

3-2 Radial detector measurements at HZP after linear tilt correction is applied. Note that all eighth-symmetric positions are extrapolated from an eighth-core symmetric radial map.

3-3 Magnitude of x and y tilts vs burnup for cycle 1.

3-4 Magnitude of x and y tilts vs burnup for cycle 2.

3-5 Radial error map between BEAVRS data without tilt-correction and CASMO/SIMULATE. RMS = 0.054.

3-6 Radial error map between BEAVRS data without tilt-correction and CASMO/SIMULATE with the inclusion of a 0.5cm water gap in southeast corner. RMS = 0.034.

3-7 Radial error map between BEAVRS data without tilt-correction and CASMO/SIMULATE with optimized water gap distribution in baffle region and between adjacent assemblies. RMS = 0.007.

3-8 Radial error map after applying linear tilt correction to BEAVRS data and to CASMO/SIMULATE with the inclusion of a 0.5cm water gap in southeast corner. This map is eighth-core symmetric and represents a conservative upper-bound for the error in each assembly when using tilt-corrected data to model time-dependent BEAVRS data. RMS = 0.006.

4-1 Cycle 1 burnup points. Full power points are indicated by green points (above 90% power). The list of full power points (in MWd/kg) are 1.02, 1.51, 2.16, 3.30, 4.61, 6.49, 7.51, 8.70, 9.80, 11.08, 12.34.

4-2 Cycle 2 burnup points. Full power points are indicated by green points (above 90% power). The list of full power points (in MWd/kg) are 0.23, 1.14, 2.11, 3.20, 4.04, 5.23, 6.52, 7.71, 8.73, 9.36, 10.43.

4-3 Core-wide normalized U-235 rate RMS error between CASMO-5/SIMULATE-3 and tilt-corrected BEAVRS data for cycle 1.

4-4 Core-wide normalized U-235 rate RMS error between CASMO-5/SIMULATE-3 and tilt-corrected BEAVRS data for cycle 2.

4-5 Reaction rates for CASMO/SIMULATE (blue) and BEAVRS (red) data for assembly D10 at 1.02, 1.51, and 2.16 MWd/kg.

4-6 Reaction rates for CASMO/SIMULATE (blue) and BEAVRS data without model bias (red) for assembly D10 at 1.02, 1.51, and 2.16 MWd/kg.

4-7 Reaction rates for CASMO/SIMULATE (blue) and BEAVRS (red) data, along with BEAVRS data with model bias subtracted out (green) for assembly D10 at 1.02, 1.51, and 2.16 MWd/kg.
4-8 Cycle 1 model bias (top) and detection uncertainty (bottom) based on CASMO/SIMULATE model. Burnups: (1.02 1.51 2.16). Assembly-weighted model bias: 0.018. Assembly-weighted detection uncertainty: 0.009.

4-9 Histogram of relative error between SIMULATE data and BEAVRS data after correcting for model bias within all assemblies over all burnups in cycle 1. RMS = 0.8%, 95% level = 1.6%.

A-1 Cycle 1 measured and linearly regressed reaction rates vs. burnup for assembly G9.

A-2 Cycle 1 RMS (top) and R-Squared (bottom) values based on applying linear model to data set of reaction rate vs. burnup for each assembly. Assembly-weighted total RMS = 0.008.

A-3 Cycle 2 RMS (top) and R-Squared (bottom) values based on applying linear model to data set of reaction rate vs. burnup for each assembly. Assembly-weighted total RMS = 0.010.

A-4 Spread level plot for linear model applied to for assembly G9 in cycle 1.

A-5 Q-Q plot for linear model applied to for assembly G9 in cycle 1.
List of Tables

2.1 Summary of 95% error results from uncertainty quantification using two methods based on reaction rate map uncertainties. .................. 37

4.1 Assembly-weighted model bias and detection uncertainty for all burnup sets in cycles 1 and 2. ......................................................... 61

4.2 Results of detection uncertainty based on three different ways of subdividing all burnups for each cycle. .............................. 63

4.3 RMS of detection uncertainty when looking at all combinations of burnup subsets of length 3 in cycle 1 and cycle 2. Outliers are marked in red. ................................................................. 64

4.4 RMS of detection uncertainty when looking at all combinations of burnup subsets of length 4 in cycle 1 and cycle 2. Outliers are marked in red. ................................................................. 64

4.5 Cycle 1 95% CI of detection uncertainty with and without outliers at 1.02 and 9.80 MWd/kg. .................................................. 65

4.6 RMS of detection uncertainty when looking at all combinations of burnup subsets of length 3 in cycle 1 when outliers at 1.02 and 9.80 MWd/kg are removed. .................................................. 65

4.7 Cycle 1 95% CI of detection uncertainty with and without outliers at 1.02 and 9.80 MWd/kg using both CASMO/SIMULATE and MPACT. .................................................. 66

4.8 RMS of detection uncertainty when looking at all combinations of burnup subsets of length 3 in cycle 1 when outliers at 1.02 and 9.80 MWd/kg are removed in CASMO/SIMULATE and MPACT. .... 67

5.1 Summary of results from uncertainty quantification using traditional methods. ................................................................. 72

5.2 Summary of results from uncertainty quantification using new methods based on time series analysis. ........................................ 72

A.1 Summary of p-values from statistical tests that test validity of linear regression model. .................................................. 84
Chapter 1

Introduction and Background

Within the field of reactor physics, increases in parallel computing capacity have ushered the development of new simulation tools that yield higher accuracy and incorporate sophisticated multiphysics phenomena. These modern methods utilize a largely available amount of computational resources to model a wide variety of geometries, material properties, and neutron transport phenomena with few approximations. Traditional techniques, on the other hand, circumvent memory and processing restrictions through homogenization schemes on coarse meshes, but such approaches lower modeling accuracy. Department of Energy projects such as Consortium for Advanced Simulations of LWR’s (CASL) [3] and Nuclear Energy Advanced Modeling and Simulation (NEAMS) [4] were therefore established to make full-core, high-fidelity modeling capabilities within current state of the art simulation software more feasible. Insights from such tools will allow for the design of current and next-generation nuclear reactors with added safety considerations and improved margins to operating limits.

1.1 The BEAVRS Benchmark

One challenge with the development of high-fidelity modeling software is the lack of full-core benchmarks able to validate new simulation methods. The BEAVRS benchmark was created by the Computational Reactor Physics Group at MIT to resolve this issue [1]. BEAVRS is a non-proprietary Pressurized Water Reactor (PWR)
depletion benchmark with two cycles of operational data that captures the detail of the entire Light Water Reactor (LWR) core. By comparing results from this benchmark to those from high-fidelity simulation tools, one can demonstrate the proper functioning of software and methods employed, ensuring that results adhere to the principles of coupled neutron transport, thermal-hydraulics, and fuel isotopic depletion. The following two sections delve into details of the benchmark specifications and operating data pertinent to this thesis.

1.1.1 Benchmark Specifications

The BEAVRS benchmark represents a 4-loop Westinghouse plant with as much detail available in open literature. Its core is octant-symmetric and contains 193 fuel assemblies, and each assembly contains a 17x17 pin lattice configuration. The core power is 3,411 MWth and the plant operates at a pressure of 2,250 psia. In cycle 1, fuel assemblies have enrichments of 1.6%, 2.4%, or 3.1%. A subset of these assemblies are shuffled for cycle 2 and fresh assemblies of enrichments of either 3.2% or 3.4% are also introduced. The loading patterns for cycle 1 and cycle 2 are given in Figures 1-1 and 1-2 respectively. Additionally, each fuel assembly contains a varying number of burnable absorbers. The absorber configuration for cycle 1 is given in Figure 1-3. Finally, Figures 1-4 and 1-5 illustrate the radial and axial zones within the reactor. All these specifications need to be incorporated into any simulation tools that try to model the physics underlying the different axial and radial zones. It should be noted that there is a water gap of 0.16 cm between the outer fuel assemblies and the baffle region. The fuel assembly pitch is 21.50 cm.

1.1.2 Operating Data

The BEAVRS reactor contains 58 assemblies that can be accessed by in-core detectors, through the central guide tubes. Figure 1-6 shows these positions, where six Uranium-235 fission chambers with varying fissile masses are used to perform measurements. When measurements are taken, multiple passes are performed occasionally within each
of the 58 assemblies to ensure accurate detector readings. All detectors pass through one common assembly for signal normalization. The detectors are inserted from the bottom through instrumentation tubes until they hit the top of the assembly. The detectors are then pulled back and take measurements of the axial fission rate over 61
Fresh 3.2 w/o U235  |  Fresh 3.4 w/o U235  
|  Shuffled Assembly  

Figure 1-2: Cycle 2 shuffling pattern, burnable absorber positions, and enrichment loading pattern of fresh assemblies [1].

axial locations. The axial fission rates can be normalized and integrated to generate a radial map of detector measurements. The exact details of this data processing are outlined below to serve as a basis for uncertainty quantification employed later on in the thesis. A full list of BEAVRS benchmark specifications and data packages
can be found at http://crpg.mit.edu/, with continuous updates to reflect improved knowledge of the core and measured data.

The first step in the process of generating radial reaction rate maps is to remove detector background signal. Next, the signal is multiplied by a gain factor to adjust the gain on the detectors. These gain factors are reported for each detector. Figure 1-7 shows the initial raw detector measurements at Hot Zero Power (HZP), while Figure 1-8 shows the measurements after correcting for background and applying gain factors.

Figure 1-8 illustrates that zero points exist where detectors were unable to make measurements. Linear interpolation/extrapolation is used between/from the nearest two points to remove these zero points. The resulting data is shown in Figure 1-9. Within each detector pass, there are minor fluctuations in core power during the
 measurement, so the detector signal is divided by power during the measurement.

Assembly J10 is the assembly where all detectors make a pass, so this is used for signal normalization purposes. Figure 1-10 shows the detector measurements in assembly J10 at HZP. It is evident from this plot that each detector has a different signal intensity due to varying Uranium-235 mass in the fission chambers, despite each detector entering the same assembly.

To account for this, each detector pass in each assembly is normalized to the signal strength of that specific detector in assembly J10. This allows all detector signals to have comparable shape functions. Figure 1-11 shows the detector signals at this
<table>
<thead>
<tr>
<th>Elevation (cm)</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>460.000</td>
<td>Highest Extent</td>
</tr>
<tr>
<td>431.876</td>
<td>Top of Upper Nozzle</td>
</tr>
<tr>
<td>423.049</td>
<td>Bottom of Upper Nozzle</td>
</tr>
<tr>
<td>421.532</td>
<td>Top of BPRA Rod Plenum</td>
</tr>
<tr>
<td>419.704</td>
<td>Top of Fuel Rod</td>
</tr>
<tr>
<td>417.164</td>
<td>Top of Fuel Rod Plenum</td>
</tr>
<tr>
<td>415.558</td>
<td>Top of Control Rod Plenum</td>
</tr>
<tr>
<td>415.164</td>
<td>Grid 8 Top</td>
</tr>
<tr>
<td>411.806</td>
<td>Grid 8 Bottom</td>
</tr>
<tr>
<td>403.778</td>
<td>Bottom of Control Rod Plenum</td>
</tr>
<tr>
<td>402.508</td>
<td>Top of Active Fuel</td>
</tr>
<tr>
<td>401.238</td>
<td>Top of Active Absorber</td>
</tr>
<tr>
<td>400.638</td>
<td>Control Rod Step 228</td>
</tr>
<tr>
<td>364.725</td>
<td>Grid 7 Top</td>
</tr>
<tr>
<td>359.010</td>
<td>Grid 7 Bottom</td>
</tr>
<tr>
<td>312.528</td>
<td>Grid 6 Top</td>
</tr>
<tr>
<td>306.813</td>
<td>Grid 6 Bottom</td>
</tr>
<tr>
<td>260.331</td>
<td>Grid 5 Top</td>
</tr>
<tr>
<td>254.616</td>
<td>Grid 5 Bottom</td>
</tr>
<tr>
<td>208.134</td>
<td>Grid 4 Top</td>
</tr>
<tr>
<td>202.419</td>
<td>Grid 4 Bottom</td>
</tr>
<tr>
<td>155.937</td>
<td>Grid 3 Top</td>
</tr>
<tr>
<td>150.222</td>
<td>Grid 3 Bottom</td>
</tr>
<tr>
<td>103.740</td>
<td>Grid 2 Top</td>
</tr>
<tr>
<td>98.0250</td>
<td>Grid 2 Bottom</td>
</tr>
<tr>
<td>41.8280</td>
<td>Bottom of Lower Absorber (AIC)</td>
</tr>
<tr>
<td>40.5580</td>
<td>Bottom of Active Absorber</td>
</tr>
<tr>
<td>40.5200</td>
<td>Grid 1 Top</td>
</tr>
<tr>
<td>39.9580</td>
<td>Control Rod Step 0</td>
</tr>
<tr>
<td>38.6600</td>
<td>Bot. of BPRA Rod</td>
</tr>
<tr>
<td>37.1621</td>
<td>Grid 1 Bottom</td>
</tr>
<tr>
<td>36.7480</td>
<td>Bottom of Active Fuel</td>
</tr>
<tr>
<td>35.0000</td>
<td>Bottom of Fuel Rod</td>
</tr>
<tr>
<td>20.0000</td>
<td>Bottom of Support Plate</td>
</tr>
<tr>
<td>0.0000</td>
<td>Lowest Extent</td>
</tr>
</tbody>
</table>

Figure 1-5: *Left*: Scale view of row 8 axial cross section, with highlighted grid spacers and partial insertion of control rod bank D to the bite position. *Right*: exhaustive list of all axial planes used in the model, excluding partial control rod insertion planes [1].

Stage. There is still some axial misalignment due to varying starting positions during recording, so the signals are subsequently aligned to grid depressions. The positions of these grid spacers are fixed, and Figure 1-12 presents the detector signals after realignment. The final step is to map the axial measurements from a grid system to a physical axial location on the active fuel. A second order spline fit is used to ensure that there are equal numbers of data points from the Top of Active Fuel (TAF) to the Bottom of Active Fuel (BAF). Figure 1-13 presents this data after the spline fit. The final measurements (no longer normalized to have the same shape functions) are shown in Figure 1-14.

With this data, axially integrated radial maps of fission reaction rates can now be created. The total sum of all signals in Figure 1-14 is computed and renormalized to be equal to the total number of assemblies (for this particular case there are 58
assemblies where measurements occurred). Axially averaging each measurement in an assembly yields a relative radial peaking factor, and Figure 1-15 depicts this factor for each assembly where measurements were taken at HZP. While the specifics of this procedure focus only on data at HZP, the same processing algorithm has been done for all burnups where data is available [1]. It has also been shown that reaction rate maps generated by core simulation software are in close agreement with those shown
Figure 1-7: Initial raw detector measurements (top to bottom) [1].

Figure 1-8: Detector measurements with gain factors applied (top to bottom) [1].

in Figure 1-15 [5].

1.2 Uses of the BEAVRS Benchmark

Since its initial release, the BEAVRS benchmark has been used by many production codes to verify whether reaction rates from these codes are in line with those processed from BEAVRS operating data [6, 7, 8, 9, 10]. BEAVRS has also been instrumental in testing whether new methodologies in computational reactor physics yield more
Figure 1-9: Detector measurements with zero points removed (top to bottom) [1].

Figure 1-10: Detector measurements within assembly J10 (top to bottom) [1].

accurate results. For example, in an EPRI study of quantifying uncertainty in reactivity burnup decrement, certain assumptions and methodologies were called into question [11]. The study used flux map data taken over 44 operational cycles of the McGuire and Catawba nuclear power plants and attempted to measure fuel reactivity burnup decrement uncertainties. However, it was questioned whether nodal diffusion calculations could provide similar accuracy compared to full-core multigroup transport calculations. Another assumption that was questioned was whether the method for calculating sub-batch reactivity could be effectively calculated simply by perturbing
fuel burnup and not other quantities such as fuel temperature. To this end, BEAVRS data was compared to data from the Studsvik Core Management System (CMS) to show that biases from the use of nodal methods over more accurate transport methods were not significant [12].
1.3 Motivation for Uncertainty Quantification

Currently, the BEAVRS benchmark is continually being improved in order to become an international benchmark for the validation of high-fidelity tools. However, a key deficiency with this benchmark is its lack of uncertainty quantification. The fundamental question of how much uncertainty lies within the operational data itself has yet to be answered. Thus, analysts using the data from the benchmark have no way of knowing whether discrepancies between operational and simulation data fit
within the tolerance of uncertainty associated with the measurement and processing of operational data.

Despite the clear need for uncertainty quantification, a major challenge is that BEAVRS measurements were performed a long time ago and very little data exists regarding uncertainties. To mitigate this shortcoming, recent work on the benchmark has thus targeted uncertainty quantification of operational data by scrutinizing all different
sources of error through each step of data gathering and processing to attribute a comprehensive range of uncertainty values for BEAVRS [2].

While this approach is the traditional way of quantifying uncertainty, the focus of this thesis is in developing an alternative way of quantifying uncertainty by implementing time series methods. More specifically, this thesis is concerned with analyzing how radially integrated operational data for each assembly varies over burnup, with hopes of comparing trends in reaction rates to those from predictive models. Using the models as a basis for how operational data should behave, this allows for an alternative means of uncertainty quantification. The ultimate goal of this work is to outline a novel methodology for uncertainty quantification, discuss the validity of assumptions surrounding this procedure, and most importantly, show that such analysis is consistent with other more conventional forms of uncertainty quantification.

1.4 Model Specifications Using CASMO/SIMULATE

The simulation tool that will be used for the bulk of this document is the Studsvik CMS code suite. This package utilizes a combination of CASMO-5, CMS-LINK, and SIMULATE-3 software to calculate core reaction rates. CASMO-5 is a lattice depletion code that computes condensed group cross sections based on the Method of Characteristics (MOC) [13]. It takes microscopic cross sections dependent on temperature and background cross sections from the ENDF-B/VII data library to generate few-group cross sections. Then, by running branch cases to cover the entire operating range of fuel/moderator temperature, burnups, and boron concentrations, associated two-group cross sections with assembly discontinuity factors (ADF’s) are calculated for each node within the reactor. CMS-LINK [14] is a linking code that generates a library of two-group cross sections and ADF’s from CASMO to feed into SIMULATE-3, the nodal diffusion solver. SIMULATE-3 runs a full-core simulation using nodal methods to generate radial reaction rates [15]. For the purposes of this thesis, full-core transport methods are not used as they are much slower and do not provide a significant reduction in errors compared to nodal diffusion methods [12].
full description of BEAVRS core models can be found in Gunow’s thesis [12].

1.5 Outline for Thesis

The remainder of this thesis describes the specifics of uncertainty quantification procedures mentioned in Section 1.3. Chapter 2 looks at two independent methods for quantifying reaction rate map uncertainties that use conventional analysis tools for assessing uncertainty during each stage of detector measurement, signal processing, and post-processing. All subsequent chapters focus on using time series analysis methods for quantifying uncertainty. Chapter 3 devises a scheme to compute the uncertainty in using tilt-corrected BEAVRS data. In Chapter 4, data from the CASMO/SIMULATE model is used to compare BEAVRS data to and ultimately compute time-dependent uncertainty. Finally in Chapter 5, the findings from the uncertainty quantification methods that use reaction rate map uncertainties and time series analysis will be compared to ultimately show that the results from these separate approaches are consistent with each other and rigorously demonstrate the uncertainty within the BEAVRS benchmark.
Chapter 2

Uncertainty in Processing and Post-Processing of BEAVRS Data

Section 1.1.2 looked at the detailed steps of processing and post-processing required to generate radial reaction rate maps. This chapter presents two different ways to quantify uncertainty within the radial maps shown in Figure 1-15. Section 2.1 first explores how to formulate the data processing and post-processing steps in more mathematical terms so that the uncertainties of each mathematical term and operation can be assessed. Section 2.2 then assigns concrete values for uncertainty and combines these results into a holistic uncertainty for each cycle. Work in this chapter has been conducted entirely by Dr. Jingang Liang and is presented for completeness and to illustrate all of the different approaches that were pursued to quantify uncertainty in the BEAVRS benchmark. Liang’s work can be found in its entirety in the NEUP BEAVRS Year 2 Report [16] as well as the conference proceedings for M&C 2017 [2].

2.1 Extracting Detector Signals and Processing Data

As mentioned in Chapter 1, the BEAVRS reactor contains 58 assemblies that can be accessed by in-core detectors through the central guide tubes. The raw measurement data for one detector in one pass includes 61 axial detector signals, background signal, gain factor of the detector, and core power. As alluded to in Section 1.1.2, the
normalized axial signal can be obtained from the detector signal by removing the background, adjusting the gain on the detector and dividing the power, as indicated by Equation 2.1.

\[
\phi_{ijk} = \frac{(D_{ijk} - B_{ij}) \times G_{ij}}{P}
\] (2.1)

\( \phi \) is the normalized axial signal, \( D \) is the detector signal, \( B \) is the background signal, \( G \) is the gain factor of the detector, \( P \) is the core power, and \( i, j, k \) indicate the spatial position of a measurement in radial assembly position \((i, j)\) and axial location \(k\).

Radial assembly reaction rate maps are obtained by integrating over all axial points, as indicated by Equation 2.2.

\[
\phi_{ij} = \sum_{k=1}^{K} \phi_{ijk}
\] (2.2)

All quantities in Equation 2.1 contribute to the overall uncertainty in radial reaction rate maps. Furthermore, all steps required for post-processing also add to the uncertainty. Each of these steps is summarized below and the methods for assessing the uncertainties from all these sources are explained in Section 2.2.

1. **Interpolation**: In some of the detector signals, zero points exist where the detector failed. These zero points are removed by performing a linear interpolation/extrapolation between/from the nearest two neighbors.

2. **Realignment**: Not all signals are aligned with each other since the starting position of the recording can differ slightly. However, signals can be realigned according to grid depressions of the signal that have fixed axial positions. These grid depressions are located at the centerlines of grids 3, 4, and 5, as shown in Figure 1-5.

3. **Spline Fitting**: Detector signals need to be put on an axial coordinate grid corresponding to points that range from the bottom to the top of the active fuel. A spline fit based on second-order polynomial functions is used to map from
measured data axial locations to an axial map with data points exactly at the Top of Active Fuel (TAF) and Bottom of Active Fuel (BAF).

2.2 Uncertainty Quantification through Theoretical Analysis of Axial Uncertainties

The uncertainty of each axial detector measurement can be expressed using Equations 2.3 and 2.4,

\[
\left( \frac{\delta \phi}{\phi} \right)_{m} = \sqrt{\left( \frac{\partial \phi}{\partial D} \cdot \delta d \right)^2 + \left( \frac{\partial \phi}{\partial B} \cdot \delta b \right)^2 + \left( \frac{\partial \phi}{\partial G} \cdot \delta g \right)^2 + \left( \frac{\partial \phi}{\partial P} \cdot \delta p \right)^2}
\]  

\[= \sqrt{\frac{\delta d^2}{(D-B)^2} + \left( \frac{\delta g}{G} \right)^2 + \left( \frac{\delta p}{P} \right)^2}
\]  

\[
\left( \frac{\delta \phi}{\phi} \right)_{ijk} = \sqrt{\left( \frac{\delta \phi}{\phi} \right)^2_{m} + \left( \frac{\delta \phi}{\phi} \right)^2_{intp} + \left( \frac{\delta \phi}{\phi} \right)^2_{align} + \left( \frac{\delta \phi}{\phi} \right)^2_{spline}
\]  

(2.3)

(2.4)

where \( \delta d \), \( \delta b \), \( \delta g \), and \( \delta p \) are the uncertainties of the detector signal, background, gain factor, and core power respectively. These sources of uncertainty contribute to the measurement uncertainty \( \left( \frac{\delta \phi}{\phi} \right)_{m} \), while \( \left( \frac{\delta \phi}{\phi} \right)_{intp} \), \( \left( \frac{\delta \phi}{\phi} \right)_{align} \) and \( \left( \frac{\delta \phi}{\phi} \right)_{spline} \) are the uncertainties introduced from interpolation, realignment and spline fitting.

2.2.1 Uncertainty from Measurement

As shown in Equation 2.3, the uncertainty in the calculation of normalized axial signal has contributions from detector signal, background, gain factor, and the core power measurements. All types of measured data are gathered and statistical analysis is used to determine the ranges and distributions of the measurements, as shown in Figure 2-1 for cycle 1. It is found that:

(1) The background values are very small, mostly provided by readings of 0 or 0.001.

Accounting for the smallest division of the detector (0.001), uncertainty of the
background can be estimated as half the smallest digit (i.e. \( \delta_b = 0.0005 \)). It should be noted that background is subtracted from detector signal and the detector signal is generally greater than 0.1 (0.41 on average), which implies from Equation 2.3 that both the effects of \( B \) and \( \delta_b \) are less than 0.1% for most cases.

(2) The gain factors are discrete values which are selected before each pass. As there are only a few well spaced-out values, it is believed that the detector error caused by using different gain factors is negligible compared to other sources, i.e. \( \delta_g \) is 0.

(3) For almost all of the measurements, the core operates at a power on the order of magnitude of 1000 MWth. As power is very important for normalization and values are reported with decimals, it can be safely assumed that its uncertainty \( (\delta_p) \) is less than 1.0 MW, which also means that \( \delta_p/P \) is under 0.1%.

(4) Axial detector signal is the final component. While the accuracy of the detector is relative to specific measurements, literature indicates that for normal reactor
applications the uncertainty is on the order of 1% [17]. Therefore, it can be concluded qualitatively that the axial detector signal dominates the measurement uncertainty.

Overall measurement uncertainty can be evaluated by performing repeated measurements and calculating the variance of these measurements. Even though the reactor core monitoring is carried out mostly once for each assembly, there are certain locations that receive multiple measurements. For example in cycle 1 of BEAVRS, there are about 180 cases that each have 2 or even 3 repeated measurements by the same detector in the same assembly. These multiple measurements are performed with nearly the same reactor core conditions such as control rod positions, boron concentration, and coolant status. Figure 2-2 is an example of multiple measurements, showing the independent axial signals as well as the mean and relative sample standard deviation (RSTD) of every axial measurement point.

![Assembly H11 by detector 3 (7 days since BOC)](image)

Figure 2-2: Multiple measurements example. Assembly H11 was measured twice by Detector 3. The average and relative sample standard deviation (RSTD) is calculated for every axial measurement point [2].

Since there are only 2 or 3 replicated measurements for each axial data point, the variance estimate is not likely to be accurate. Thus, gathering the data over all multiple cases and averaging the data are necessary to obtain a reliable uncertainty
estimate. Here it is assumed that the multiple measurement cases with similar mean value have similar uncertainty. Therefore the data points can be grouped by amplitude and an average uncertainty can be estimated for each group. To make the estimate more conservative, a 95% confidence value is adopted as the resulting uncertainty. During these calculations, all the data is sorted by group and the value at the 95% position is selected. Here, a group is defined as the measurement signal interval where an equal number of points lie.

There are 10,725 multiple measurements in cycle 1 and they are divided into 30 groups by signal amplitude, with equal number of data points in each group. 30 groups were chosen to ensure an adequate level of resolution to capture amplitude variations within the entire range of signals, while still maintaining enough measurements per group for accurate statistics. There are roughly 360 and 250 measurements per group in cycles 1 and 2 respectively. The 95% confidence values are calculated for each group, thus a lookup table of signal ranges and measurement uncertainties is obtained, as shown in Figure 2-3. This lookup table will be applied to all detector signals.

As can be seen in Figure 2-3, the axial measurement uncertainty is generally around 2−12% and is dependent on signal amplitude. Generally, the greater the signal the smaller the uncertainty.

2.2.2 Uncertainty from Interpolation

To analyze the uncertainty interpolation, realignment, and spline fitting, a method of observing the variation before and after the processing is used. Interpolation is performed when a single data point is unrecorded. To estimate the error of interpolated data, points that were properly recorded were simply eliminated one-by-one and then the axial relative error was compared with the recorded data. Figure 2-4 displays all the interpolation errors and their averages along with axial locations. It is observed that the interpolation error is dependent on location and is greater near endpoints and grid spacers. Here again the 95% confidence estimate is used for each location. The 95% confidence value for each axial position is collected as a lookup table to estimate the uncertainty of every interpolation performed during processing.
Figure 2-3: Axial signal uncertainty from all multiple measurements in cycle 1. Top: A plot of the average and relative sample standard deviation of all multiple measured data points. Bottom: A plot that divides the data points into groups and calculates the 95% confidence values for all groups to represent as a measurement uncertainty table [2]. While the overall distribution is not normally distributed, statistics within each group follows a normal distribution.

2.2.3 Uncertainty from Axial Realignment

Realignment of axial signals is carried out such that axial signals are provided over the active fuel length. The positions of the axial data are moved up or down in realignment, with the lost edge points calculated using extrapolation. Axial measurements are realigned by one or two axial positions, and in some rare situations three axial positions. Here, realignment occurs based on shifting the axial points where grid depressions occur to the centerlines of grids 3, 4, and 5, defined in Figure 1-5.

Two sources of error stem from realignment. The first one is from extrapolation of end points. A similar method as interpolation uncertainty is used to estimate the error of these extrapolations, where original measured data is compared to extrapolated data. Figure 2-5 shows the extrapolation errors gathered by the 6 grid positions as well as the 95% confidence values of these errors. Again, this data will be used as a lookup table to estimate error of axial points which are extrapolated when realignment is
Figure 2-4: A representation of axial interpolation uncertainty. *Top:* Interpolation errors along with axial locations. *Bottom:* Interpolation uncertainty table using 95% confidence values for all locations [2].

Secondly, even after all the signals are realigned, the measured locations themselves can be erroneous due to the fluctuations in starting positions and the detector moving speeds. During realignment, it is found that more than half of the assemblies are shifted by one or more axial measured grids. To simplify the problem, it is assumed that at 95% confidence, the uncertainty of the measurement position is within one measured grid length. In other words, every measurement point can be wrongly recorded as much as its upper or lower grid point. Therefore, the positional uncertainty of each signal can be calculated as the larger error between the current point and its two neighboring grid points. It should be noted the positional error is sensitive to the location and the variation of the signal. In a flat region like the middle core, the signal varies by about 1% within one grid, while around the endpoints this number can be as much as 30%. The realignment uncertainty is considered as the combination of extrapolation error and positional error.
2.2.4 Uncertainty from Spline Fitting

Spline fitting is used to put the detector signals on an axial coordinate grid corresponding to points that range from the bottom to the top of the active fuel. The error introduced in spline fitting is found negligible because the second order spline fit is quite accurate and the errors are less than $10^{-10}$. In other words, $(\delta \phi / \phi)_{\text{spline}} \approx 0$.

2.2.5 Uncertainty of Axially Integrated Radial Data

Finally, the uncertainties of all axial signals can be quantified by calculating all independent uncertainties at each processing and post-processing step using lookup tables and combining them together using Equation 2.4. Specifically, the following steps will be performed for every axial signal.

1. The measurement uncertainty $(\delta \phi / \phi)_m$ is determined according to the amplitude of calculated axial data, based on Figure 2-3.

2. If this data point is interpolated, an interpolation error $(\delta \phi / \phi)_{\text{interp}}$ is determined
according to its location on the lookup table obtained from Figure 2-4.

(3) If this data point is realigned, an extrapolation error \( \left( \frac{\delta \phi}{\phi} \right)_{align} \) is determined according to its location. Furthermore, the positional uncertainty is calculated as the larger error between the current signal and its two neighboring points.

(4) The square root of sum of squares of all uncertainties is calculated as \( \left( \frac{\delta \phi}{\phi} \right)_{ijk} \) for each data point according to Equation 2.4.

Uncertainty of axially integrated radial assembly data can be evaluated by accounting for the errors of all axial points in one assembly, as indicated by Equation 2.5,

\[
\left( \frac{\delta \phi}{\phi} \right)_{ij} = \sqrt{\sum_{k=1}^{K} \left( \delta \phi \right)_{ijk}^2 / \phi_{ij}}
\]  

(2.5)

where \( i \) and \( j \) represent the radial assembly position and \( k \) the axial location.

The uncertainties of all assembly data at all burnups are calculated this way. Figure 2-6 gives the full core radial detector measurements together with the calculated uncertainties under HZP conditions in cycle 1. Furthermore, by gathering all assembly uncertainties in the whole cycle, it is found the average uncertainty of radial measurements is 1.0% for both cycle 1 and cycle 2 and the 95% confidence value is 1.4%. Average uncertainty refers to the root mean square value (RMS), while the 95% confidence value is the value below which 95% of the underlying uncertainty data lies.

### 2.3 Uncertainty Quantification through Multiple Measurements

Multiple measurements present within BEAVRS data can also be used to quantify uncertainty of radial data in a different way. Similar to the treatment of multiple axial signals, all multiple measurement cases of radial data are collected and statistics are computed to estimate uncertainty of radial data, as shown in Figure 2-7. There are 179 cases of multiple measurements in cycle 1. The 95% confidence value is 1.8%.
Figure 2-6: Radial assembly measurements with uncertainties calculated from axial uncertainties at HZP in Cycle 1. The top number is normalized assembly signal while the bottom number is its uncertainty [2].

### 2.4 Motivation for Time Series Analysis

This chapter presents two separate methods for uncertainty quantification derived from reaction rate map uncertainties. Table 2.1 provides the 95% confidence uncertainties for both methods in cycles 1 and 2, and it can be seen that both approaches demonstrate consistent results.
Figure 2-7: Distribution of radial data uncertainty calculated from axial uncertainties in cycle 1 [2].

<table>
<thead>
<tr>
<th>Method of Uncertainty Quantification</th>
<th>Theoretical Analysis of Axial Uncertainties (Axially Integrated)</th>
<th>Multiple Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle 1</td>
<td>1.4%</td>
<td>1.8%</td>
</tr>
<tr>
<td>Cycle 2</td>
<td>1.4%</td>
<td>1.5%</td>
</tr>
</tbody>
</table>

Table 2.1: Summary of 95% error results from uncertainty quantification using two methods based on reaction rate map uncertainties.

The uncertainty quantification work that has been performed in this chapter has dealt with analyzing the sources of uncertainty at individual burnups, where each burnup step is regarded as independent of neighboring burnup steps. However, the following chapters aim to characterize how reaction rates vary over specific time intervals using predictive models in order to determine whether calculated reaction rates follow any observable trend. By fitting BEAVRS data to such trends, any resulting deviation can be regarded as an alternative method for uncertainty quantification.
Chapter 3

Uncertainty in Using Tilt-Corrected BEAVRS Data

As mentioned in Chapter 2, the work from here onward will deal with fitting trends over burnup of radially integrated reaction rates that have been calculated for BEAVRS. However, looking at Figure 1-15, this data is not eighth-core symmetric despite a symmetric core loading pattern. While there is some asymmetry in the location of instrument tubes and as-built masses, as seen in Figure 1-6, this alone does not describe the significant tilt in the data. This tilt was first described in detail by Sykora in his Master’s thesis, where he devises an algorithm to remove this tilt to yield eighth-core symmetric reaction rates [18]. The magnitude of this tilt is not fixed, however, and slowly decreases over burnup. Eliminating the tilt is essential in the process of fitting the CASMO/SIMULATE model to BEAVRS data, which is explored in Chapter 4. This is because simulation tools will produce symmetric results given a symmetric core loading pattern and cannot arbitrarily impose a tilt to mimic that observed in BEAVRS data. Thus, tilt correction allows for a more accurate comparison between operational and simulated data, but artificially masks an un-modeled phenomenon within the operating data. The exact amount of added uncertainty from assuming a linear tilt correction is the focus of this chapter. While other tilt distribution types were looked at, it was found that a linear tilt performed best in terms of modeling the tilt observed within operating data. Section 3.1 explores
the process of identifying the best x-y plane to fit BEAVRS data, and Section 3.2
investigates work by Sykora in trying to mimic such a linear tilt by assuming a 0.5
cm water gap between the baffle and assemblies in the southeast corner. While this
is an apt starting point for quantifying uncertainty in using tilt-corrected BEAVRS
data, Section 3.3 expands upon this work to devise a more comprehensive method
for simulating the tilt observed in BEAVRS data. Finally, Section 3.4 uses the radial
map that results from this revised approach as a basis for evaluating tilt-correction
uncertainty.

3.1 Generation of Tilt-Corrected Data

Asymmetry in the calculated measured fission rates are corrected by assuming that
deviations follow a purely linear tilt. This linear tilt is determined by perturbing
x-y tilt coefficients and finding the plane that best fits measured data. This plane
minimizes RMS between symmetric detector fission rates relative to the plane, and
octant-core symmetric “tilt-corrected data” can be generated by subtracting the tilt of
this plane from measured data. All modeled data will be compared to this tilt-corrected
data. Figure 3-1 shows the original BEAVRS measured data at HZP, while Figure
3-2 illustrates what this data looks like after tilt-correction. Viewing the magnitude
of the tilt over burnup also highlights how the effect of radial asymmetry decreases
with time. This can be seen in Figures 3-3 and 3-4 for cycle 1 and 2 respectively. The
source of this behavior is not known exactly, but the leading hypothesis is that uneven
water gaps during core loading is causing this irregularity [19]. Typically, core loading
is performed in a crescent pattern starting from one corner and working around to
the opposite corner. As a result, bundles could have leaned against the baffle during
insertion, causing uneven gaps to occur in opposite corners of the core. As the reactor
heats up, symmetric water gaps are restored through fuel swelling under irradiation.
This could explain the presence of a large tilt at HZP that dissipates with burnup
as observed in the BEAVRS benchmark. To test this hypothesis, a water gap test
was conducted by Sykora to determine whether adding a 0.5 cm water gap in the
southeast corner between the baffle and assemblies would mirror the observed tilt in BEAVRS data [18]. The results from this test are included in Section 3.2.

Figure 3-1: Radial detector measurements at HZP (axially integrated) [1].
3.2 Initial Gap Test to Mimic Tilt in BEAVRS Data

A 0.5 cm water gap can be modeled in SIMULATE between the fuel assemblies and the baffle in the southeast corner of the core. To illustrate the effect of an updated model which includes this water gap on overall modeling accuracy, a radial error
Figure 3-3: Magnitude of x and y tilts vs burnup for cycle 1.

Figure 3-4: Magnitude of x and y tilts vs burnup for cycle 2.

map before and after the water gap inclusion at HZP is shown in Figures 3-5 and 3-6 respectively\(^1\). While the core-wide RMS reduces dramatically, this simple water gap model does not wholly explain the cause of the tilt in BEAVRS data. A major reason for this is that the addition of the water gap induces an exponential tilt which helps reduce the errors on the periphery of the core but still adds significant errors in

\(^1\)The radial error map shown in Figure 3-6 after adding a 0.5 cm water gap differs slightly from the one found in Sykora’s Master’s thesis because of updated BEAVRS specifications since the publishing of his findings. Further discrepancies also arise due to the fact that the SIMULATE-3 nodal diffusion solution was used instead of the CASMO-5 MxN full-core transport solution used by Sykora.
the core center, where a linear tilt is more suitable than an exponential one. Thus, accounting for varying water gaps throughout the core and not just at the edge will allow for tuning of the water gap to compensate for this phenomenon. Furthermore, Sykora finds that keeping a fixed water gap through depletion results in higher errors due to the resulting exponential tilt over-correcting the real tilt in BEAVRS data [18]. This suggests that the gap must vanish or reduce with burnup. A key element in tilt-correction uncertainty quantification therefore is to introduce more degrees of freedom in water gap distribution to reduce RMS and to match the BEAVRS radial map more closely to simulated results. This approach will be pursued in Section 3.3.

3.3 Methodology for Tilt-Correction Uncertainty Quantification

In order to improve Sykora’s water gap test, now water gaps between adjacent assemblies will also be varied to induce a tilt in SIMULATE that further replicates the one observed in BEAVRS data at HZP. Doing so hopefully will counteract the effect of the exponential tilt seen by varying just the reflector-assembly gaps. The presence of different water gaps throughout the core would affect moderation within each assembly and provide additional parameters to bring the tilt generated in SIMULATE closer to that detected in BEAVRS data. Thus, the task of tilt-correction uncertainty quantification is formulated into a large-scale optimization problem, whereby the objective function is a minimum RMS between BEAVRS data (not tilt corrected) and SIMULATE reaction rate data, and the optimization parameters within SIMULATE are the water gaps between adjacent assemblies as well as the water gap between outer assemblies and the baffle. Since the generation of SIMULATE reaction rate maps don’t follow a simple mathematical operator, traditional optimization methods that guarantee the location of a global minimum cannot be used. Furthermore, since there are a large number of inter-assembly gaps and assembly-baffle gaps that can be modeled, a brute-force approach of testing all possible gap combinations, even for a
narrow range of gap perturbations, is highly unfeasible.

For this process, the parameters for 129 fuel regions and 64 reflector regions are perturbed². Water gaps between outer assemblies and the baffle can take on any

²All fuel assemblies with enrichments of 1.6% and 2.4% are perturbed. 3.1% enriched assemblies maintain a fixed assembly pitch of 21.50 cm. These assemblies are not included as part of the optimization simply to reduce the number of optimization parameters and also because it is believed that perturbations in the reflector region water gaps can compensate for any large errors in the 3.1% enriched assembly regions, since these assemblies are all located on the core periphery. Moreover, SIMULATE discretizes the reflector region into 64 nodes, adding a larger amount of reflector material where the neutron shield panel is present.
Figure 3-6: Radial error map between BEAVRS data without tilt-correction and CASMO/SIMULATE with the inclusion of a 0.5cm water gap in southeast corner. RMS = 0.034.

...values between 0.00 cm to 0.85 cm, in 0.01 cm increments, while the inter-assembly pitch is varied between 21.42 cm to 21.58 cm, in 0.01 cm increments. 21.42 cm represents the lower bound where there is no inter-assembly water gap, and 0.85 cm and 21.58 cm are chosen empirically based on the fact that any water gaps larger than these amounts have negligible effects on reducing RMS for any single assembly.

Initial testing focused on perturbing just the gaps in the reflector region to reduce RMS as much as possible without altering inter-assembly pitches. All reflector regions were...
grouped into octants and perturbed with very coarse parameter intervals to reduce computational constraints for an optimization problem that takes exponential-time to compute. It was found that lower RMS values were attained when gaps were 0.08 cm in the northwest region, 0.80 cm in the southwest region, and 0.22 cm in southwest and northeast regions. These results are consistent with Sykora’s initial water gap test, which found that large water gaps in the southeast reflector regions and moderate water gaps in other quadrants tended to lower RMS.

Now, with this approximate water gap distribution in the reflector region, it is time to focus on the fuel regions. Given the sheer number of fuel regions that can be perturbed, it is now necessary to impose additional constraints and changes to the optimization to reduce runtime from one that is exponential to one that is polynomial in nature. In order to achieve this, an initial gap distribution is selected. At each iteration, each of the 129 assemblies is perturbed by ten varying water gaps. The gap that minimizes RMS for that assembly is stored. After a single assembly perturbation, the gap is restored to its initial gap distribution before moving on to the next assembly to perturb. In this manner, the single assembly gap perturbation that leads to a minimum RMS over all 129 assemblies is found and fixed for the remainder of the algorithm. In the subsequent iteration, 128 assemblies are now perturbed and the single assembly gap perturbation that minimizes RMS is found and fixed for that specific assembly. This process is repeated for all remaining unfixed assemblies until there are no more remaining assemblies to perturb or the RMS does not reduce from the previous iteration to the current iteration. Suppose each assembly can be initially perturbed by 10 different possible water gaps. Then a simple upper bound calculation for amount of time it would take for this entire optimization would be,
Total SIMULATE Runs \[= \left( 129 \text{ Perturbed Assemblies} \times \frac{10 \text{ Perturbations}}{\text{Assembly}} \right) + \]
\[\left( 128 \text{ Perturbed Assemblies} \times \frac{10 \text{ Perturbations}}{\text{Assembly}} \right) + \ldots + \]
\[\left( 2 \text{ Perturbed Assemblies} \times \frac{10 \text{ Perturbations}}{\text{Assembly}} \right) + \]
\[\left( 1 \text{ Perturbed Assembly} \times \frac{10 \text{ Perturbations}}{\text{Assembly}} \right) \]
\[= 83,850 \text{ SIMULATE Runs} \]

Total Runtime \[= 83,850 \text{ SIMULATE Runs} \times \frac{3 \text{ Seconds}}{\text{SIMULATE Run}} \]
\[= 2.91 \text{ Days} \quad (3.1) \]

where this case would only be achieved if all gaps of the initial gap distribution were changed and RMS kept decreasing in each iteration. This is a much favorable alternative to testing all possible combinations of gap distributions within the 129 assemblies. In the latter case, this becomes an exponential problem with \(10^{129}\) possibilities. A detailed description of the algorithm used to optimize the water gap distribution for a certain number of nodal regions is shown in Algorithm 3-1. It should be noted that that the term varying refers to a Boolean datatype specifying whether a node should be perturbed or whether it will have a fixed gap for the remainder of the optimization.

Once an optimized water gap distribution results from perturbing the 129 fuel assemblies, the focus is shifted back to the reflector nodes. In the process of improving the water gap distribution within the assemblies, the reflector gaps were kept fixed, but now the reflector gaps can be varied while keeping the optimized fuel assembly gap distribution from the previous optimization fixed to attain a new minimum RMS. The same polynomial-time approach as Algorithm 3-1 is used to optimize the water gap distribution within the reflector nodes. Iterating back and forth between varying just the fuel assembly nodes and varying just the reflector nodes, a final optimized error map is generated, where now perturbing the gap in any single nodal region does
Algorithm 3-1 Algorithm for Optimizing Water Gap Distribution Within SIMULATE

1: Assign reference gap distribution \( \triangle \) Could come from a previous optimization
2: \( \text{RMS}_{\text{base}} \leftarrow \text{RMS from reference gap distribution} \)
3: Set all nodes that will be perturbed as varying
4: Assign all gap perturbations for each varying node
5: \textbf{while} At least one node is varying \textbf{do}
6: \( \text{RMS}_{\text{curr}} \leftarrow \text{RMS}_{\text{base}} \) \( \triangleright \) Minimum RMS from current iteration
7: \textbf{for all} node in nodes \textbf{do}
8: \textbf{if} node is varying \textbf{then}
9: Retrieve all gap perturbations for node
10: \textbf{for all} gap perturbation in gap perturbations \textbf{do}
11: Set node gap to gap perturbation
12: Run SIMULATE with this node gap
13: \( \text{RMS}_{\text{temp}} \leftarrow \text{RMS from this SIMULATE run} \)
14: \textbf{if} \( \text{RMS}_{\text{temp}} < \text{RMS}_{\text{curr}} \) \textbf{then} \( \triangleright \) New minimum RMS found
15: Store node and gap perturbation
16: \( \text{RMS}_{\text{curr}} \leftarrow \text{RMS}_{\text{temp}} \)
17: \textbf{end if}
18: \textbf{end for}
19: Reset node gap to value from reference case \( \triangleright \) See Step 1
20: \textbf{end if}
21: \textbf{end for}
22: \textbf{if} \( \text{RMS}_{\text{curr}} = \text{RMS}_{\text{base}} \) \textbf{then} \( \triangleright \) No new minimum RMS found in iteration
23: Break from while loop
24: \textbf{else} \( \triangleright \) Update minimum RMS and fix node gap
25: \textbf{set} node that yields \( \text{RMS}_{\text{curr}} \) as fixed \( \triangleright \) No longer perturb this node
26: \textbf{set} node gap to perturbation value that yields \( \text{RMS}_{\text{curr}} \)
27: \( \text{RMS}_{\text{base}} \leftarrow \text{RMS}_{\text{curr}} \)
28: \textbf{end if}
29: \textbf{end while}

not lower RMS any further. This error map is shown in Figure 3-7, which has an RMS of 0.7%. Beyond this point, the errors are very sensitive to a single assembly perturbation. Moreover, SIMULATE requires that there can only be 200 unique nodal segments, so this inhibits further optimization using gap perturbation increments finer than 0.01 cm.

It should be noted that while opting for a polynomial-time optimization over an exponential-time optimization saves tremendous runtime while exploring a wide range of perturbation combinations, a key shortcoming of this work is that this approach does not guarantee a global minimum. During each outer iteration, when an assembly gap
Figure 3-7: Radial error map between BEAVRS data without tilt-correction and CASMO/SIMULATE with optimized water gap distribution in baffle region and between adjacent assemblies. RMS = 0.007.

is fixed the implicit assumption is that this fixed gap is part of the final optimized gap profile. It ignores any possibility of gap perturbations within two different nodes that might have higher RMS individually but together contribute to an overall lower RMS. While each outer iteration in Algorithm 3-1 ensures a lower RMS, each successive perturbation could drive the final solution closer to a local minimum rather than a global minimum. However, for the purposes of this work, achieving a global minimum is not absolutely critical since the local minimum that was found in Figure 3-7 was
within the bounds of a 1-sigma deviation of the measurement uncertainties outlined in Chapter 2.

It should be noted here that a key assumption in the generation of this radial map is that predictive models are capable of capturing reactor behavior for small burnup ranges. The closer that these models can be brought to mimic BEAVRS data, the stronger the argument that the behavior of operating data is accurately being modeled by simulation tools. Since the exact source of the tilt in BEAVRS data is not known and there is relative lack of certainty in the inter-assembly gap due to imperfect core loading, incorporating such gap variations for modeling purposes could be justifiable, especially given that the magnitude of these gap perturbations is quite minute. Furthermore, analysis is restricted to quantifying the uncertainty of the linear tilt at HZP, where the magnitude of this tilt is largest and represents a conservative upper-bound in uncertainty levels.

### 3.4 Evaluation of Tilt-Correction Uncertainty

With this tilt-induced SIMULATE map generated from a varying water gap distribution, there now exist two sets of comparable data between BEAVRS and SIMULATE to assess the added uncertainty of imposing a linear tilt correction to the data sets. The following procedure will be used to quantify such uncertainty:

1. The linear planar tilt correction is applied to the BEAVRS case at HZP for cycle 1. The resulting map is shown in Figure 3-2.

2. Likewise, the linear planar tilt correction is applied to the optimized SIMULATE map generated by perturbing the water gap profile at HZP. This map represents the reference case that tilt-corrected HZP BEAVRS data will be compared to.

3. The resulting radial maps from Steps (1) and (2) are now octant core-symmetric. The two radial maps are collapsed to an eighth-core and relative errors at each octant-symmetric position are calculated to assess the underlying uncertainty in using tilt-corrected BEAVRS data for each assembly.
Following this procedure, the eighth-core collapsed error maps generated after Step (3) is shown in Figure 3-8. This map represents the resulting error in each assembly after imposing a linear tilt correction on both BEAVRS data as well as SIMULATE data with an induced gap that mimics the tilt in BEAVRS data.

![Error Map](image)

Figure 3-8: Radial error map after applying linear tilt correction to BEAVRS data and to CASMO/SIMULATE with the inclusion of a 0.5cm water gap in southeast corner. This map is eighth-core symmetric and represents a conservative upper-bound for the error in each assembly when using tilt-corrected data to model time-dependent BEAVRS data. RMS = 0.006.

Thus, when computing overall time-dependent uncertainty for each assembly by imposing a time-dependent model to BEAVRS data, Equation 3.2 will be used,

\[
\left( \frac{\delta \phi}{\phi} \right)_{ij, \text{time-dep}} = \sqrt{\left( \frac{\delta \phi}{\phi} \right)_{ij, \text{detection}}^2 + \left( \frac{\delta \phi}{\phi} \right)_{ij, \text{tilt-corr}}^2}
\]  

(3.2)

where \((\delta \phi/\phi)_{ij, \text{time-dep}}\) represents the time-dependent uncertainty of each radial as-
assembly position, \((\delta_{\phi}/\phi)_{ij,\text{detection}}\) represents the error induced from fitting a simulation model to assembly-level BEAVRS data, and \((\delta_{\phi}/\phi)_{ij,\text{tilt-corr}}\) represents the conservative upper-bound error within each assembly that stems from assuming a linear tilt-correction to BEAVRS data. In other words, overall time-dependent uncertainty has a contribution from error that is rooted within assuming a model to fit time-dependent data as well as from an un-modeled phenomenon that accounts for an imperfect replication of the tilt observed within BEAVRS data. Chapter 4 focuses on the CASMO/SIMULATE model to fit BEAVRS data to and outlines a methodology for calculating \((\delta_{\phi}/\phi)_{ij,\text{detection}}\). The value of \((\delta_{\phi}/\phi)_{ij,\text{tilt-corr}}\) for each assembly, on the other hand, is given by the errors in Figure 3-8.

3.5 Interpretation of Results

To summarize the work in this chapter, first BEAVRS data was assessed over burnup and it was found that imposing a linear tilt correction was necessary for closer comparison between BEAVRS and simulation data. However, this step introduces added uncertainty due to the fact that now the BEAVRS data set is altered in a way that is not accounted for in simulation tools. Thus, to quantify the amount of bias introduced in tilt correction, a comparable SIMULATE map with an induced tilt is generated. This tilt is produced to mimic the BEAVRS tilt as closely as possible, and this is done by varying the water gap between adjacent assemblies and between outer assemblies and the baffle region. With both BEAVRS and SIMULATE maps now bearing similar tilts, a linear tilt correction is applied to both radial profiles at beginning of cycle and the resulting eighth-core symmetric error map can be used in Equation 3.2 to compute the contribution of time-dependent error from assuming a linear tilt-correction in BEAVRS data. This uncertainty will be accounted for in Chapter 4, where data from a simulation model will be compared to BEAVRS data to compute overall time-dependent uncertainty.

While the work in this chapter could be extended to multiple burnups by accounting for depletion, this effort will not be examined simply because there is no way of
knowing how the water gaps vary with time. Each burnup step provides even more degrees of freedom to optimize over, making the problem even more intractable. There is no basis from operational data to confirm depletion behavior of these gaps, and thus strong assertions about the nature of the tilt in BEAVRS data with respect to time cannot be made. HZP is chosen as the focus for this chapter mainly because the tilt is highest at this point and thus the uncertainty introduced by imposing a tilt-correction would also result in the most conservative value.
Chapter 4

Time Dependent Uncertainty in the BEAVRS Benchmark Using the CASMO/SIMULATE Model

The motivation for computing time-dependent uncertainty can be understood by seeing how operational data behaves over time. Assuming that at each burnup point, there is a constant but independent uncertainty associated with each axially-integrated reaction rate for a particular assembly, the goal for this chapter is to figure out whether the time-varying behavior of reaction rates for each assembly follow an observable trend. If so, this trend is characterized and any deviation from this behavior can be attributed to an additional measure of time-dependent uncertainty. To this end, simulated reaction rates from CASMO-5 lattice codes and SIMULATE-3 nodal diffusion simulator will serve as an additional basis for comparison. Trends in two cycles of operation are considered, and as explained in Chapter 3, tilt-corrected BEAVRS data is used to fit linear trends.

Analysis from CASMO/SIMULATE is suitable, however, only when reactors are operating near steady-state conditions. Thus, the time-dependent analysis for this chapter is restricted to looking exclusively at burnup points that are full-power points, defined as those burnup points above 90% rated power. Figures 4-1 and 4-2 show the power history for cycle 1 and 2 respectively, with the green points representing...
burnups that are full power points. This entire burnup range of full power points will be subdivided into smaller subset of burnups, as the highly volatile power history makes it difficult to model reaction rates effectively over a very long burnup.

Figure 4-1: Cycle 1 burnup points. Full power points are indicated by green points (above 90% power). The list of full power points (in MWd/kg) are 1.02, 1.51, 2.16, 3.30, 4.61, 6.49, 7.51, 8.70, 9.80, 11.08, 12.34.

Figure 4-2: Cycle 2 burnup points. Full power points are indicated by green points (above 90% power). The list of full power points (in MWd/kg) are 0.23, 1.14, 2.11, 3.20, 4.04, 5.23, 6.52, 7.71, 8.73, 9.36, 10.43.

Section 4.1 begins by examining what core-wide RMS between SIMULATE and BEAVRS data looks like in order to provide a holistic perspective of how errors behave.
over burnup. This transitions into a narrower analysis of assembly-level behavior in Section 4.2, where it is found that simulations overpredict reaction rates by a small but persistent discrepancy labeled as model bias. The remaining detection uncertainty after correcting for model bias is evaluated over the entire burnup range in Section 4.3 in an attempt to produce a core-level error heuristic over the entire cycle. Section 4.4 tests the assumptions made during this analysis, while Section 4.5 verifies that the results are not dependent on the model used by running the same tests with data from an alternative simulation model to compare against results from the CASMO/SIMULATE model. Data from this model was provided by the CASL team [20]. Section 4.6 combines detection uncertainty with uncertainty from using tilt-corrected data to find overall time-dependent uncertainty, and finally Section 4.7 summarizes key results and findings from the chapter. This thesis also considers using the linear regression model as an alternative method to replicate time-dependent BEAVRS reaction rates. Details of this work can be found in Appendix A.

4.1 Visualization of Core-wide RMS

Time series analysis can be conducted at the core level by observing how RMS between BEAVRS and SIMULATE maps vary at each burnup point. This is shown in Figure 4-3 for cycle 1 and in Figure 4-4 for cycle 2. From these graphs it is evident that core-wide RMS essentially decreases over burnup for both cases, and that the data for cycle 2 is much smoother than for cycle 1 due to the smoother power history in cycle 2. For cycle 1, there is reason to believe that burnup points 1.02 MWd/kg and 9.80 MWd/kg are outliers. The measurement readings at 9.80 MWd/kg happened during temporary shutdowns, while the recordings at 1.02 MWd/kg occurred while the reactor was still ramping up and had not yet attained full power. These observations will become especially important in Section 4.4, where it is shown that analysis conducted with the outlier burnup points in cycle 1 yields erratic results since the state of the core is not well characterized during these transition periods.
Figure 4-3: Core-wide normalized U-235 rate RMS error between CASMO-5/SIMULATE-3 and tilt-corrected BEAVRS data for cycle 1.

Figure 4-4: Core-wide normalized U-235 rate RMS error between CASMO-5/SIMULATE-3 and tilt-corrected BEAVRS data for cycle 2.

4.2 Characterization of Model Bias

The focus will now shift to assembly-level CASMO/SIMULATE data. As aforementioned, only a subset of burnups are going to be examined at a time, due to the unstable power history. Figure 4-5 plots reaction rates for CASMO/SIMULATE and BEAVRS data for assembly D10 at the first three burnups of 1.02, 1.51, and 2.16 MWd/kg in cycle 1. Looking at this region, it is clear that the two plots exhibit a
similar shape but are offset by some amount. Defining this offset as model bias, the goal is to overlay the BEAVRS data onto the CASMO/SIMULATE data, and then measure how much noise there is between this new data set and CASMO/SIMULATE. This resulting noise can be quantified as a measure of detection uncertainty. Only assemblies that have a complete data set for these three burnups are used.

**Figure 4-5:** Reaction rates for CASMO/SIMULATE (blue) and BEAVRS (red) data for assembly D10 at 1.02, 1.51, and 2.16 MWd/kg.

Thus, the methodology that is pursued is to calculate relative percent error at each burnup and average this value across all burnups to get an estimate of the average deviation between detector readings and simulated reaction rates. For each burnup, this average deviation is subtracted and new detector readings are extrapolated based on this new percent error. Figure 4-6 shows the new extrapolated detector readings that are calculated once average relative error is subtracted out. The new BEAVRS data curve is basically a version of the original data that is overlaid onto CASMO/SIMULATE data. With this new curve, RMS can be quantified and deemed as detection uncertainty. Model bias in this case is defined as the RMS value of percent errors between the original BEAVRS data and CASMO/SIMULATE data. For assembly D10, model bias is 0.6%, while detection uncertainty is 0.1%.

By extending this methodology for all assemblies within the burnup range of 1.02, 1.51, and 2.16 MWd/kg, both model bias and detection uncertainty can be quantified for all
Figure 4-6: Reaction rates for CASMO/SIMULATE (blue) and BEAVRS data without model bias (red) for assembly D10 at 1.02, 1.51, and 2.16 MWd/kg.

Figure 4-7: Reaction rates for CASMO/SIMULATE (blue) and BEAVRS (red) data, along with BEAVRS data with model bias subtracted out (green) for assembly D10 at 1.02, 1.51, and 2.16 MWd/kg.

assemblies. Figure 4-8 shows the results for all assemblies within the symmetric eighth-core. Once again, an RMS value that weighs both model bias and detection uncertainty by the number of symmetric positions for that specific assembly is calculated. RMS for model bias for the entire core is 1.8%, while the RMS for detection uncertainty is 0.9%.
Figure 4-8: Cycle 1 model bias (top) and detection uncertainty (bottom) based on CASMO/SIMULATE model. Burnups: (1.02 1.51 2.16). Assembly-weighted model bias: 0.018. Assembly-weighted detection uncertainty: 0.009.

4.3 Quantifying Detection Uncertainty Over Entire Burnup Range

Assuming that burnup sets with non-overlapping points are independent of each other, SIMULATE data is now fitted for the remaining 8 burnup points that were not included in the first burnup set (1.02, 1.51, 2.16). The remaining 8 points are divided into two sets of four burnups so that SIMULATE data is compared to the burnup sets (3.3 4.61 6.49 7.51) and (8.7 9.8 11.08 12.34). The results for assembly-weighted core-wide model bias and detection uncertainty are summarized for all burnup ranges in Table 4.1. For cycle 2, the entire burnup range is divided up in a similar manner,
where core model bias and detection uncertainties are computed for the burnup sets
(0.23, 1.14, 2.11), (3.20, 4.04, 5.23, 6.52), and (7.71, 8.73, 9.36, 10.43). The results for
cycle 2 are also given in Table 4.1.

<table>
<thead>
<tr>
<th>Cycle 1 Burnup Points</th>
<th>Core-Wide Model Bias (RMS)</th>
<th>Core-Wide Detection Uncertainty (RMS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1.02, 1.51, 2.16)</td>
<td>1.8%</td>
<td>0.9%</td>
</tr>
<tr>
<td>(3.30, 4.61, 6.49, 7.51)</td>
<td>1.1%</td>
<td>0.6%</td>
</tr>
<tr>
<td>(8.70, 9.80, 11.08, 12.34)</td>
<td>1.4%</td>
<td>0.9%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cycle 2 Burnup Points</th>
<th>Core-Wide Model Bias (RMS)</th>
<th>Core-Wide Detection Uncertainty (RMS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0.23, 1.14, 2.11)</td>
<td>1.6%</td>
<td>0.6%</td>
</tr>
<tr>
<td>(3.20, 4.04, 5.23, 6.52)</td>
<td>1.2%</td>
<td>0.3%</td>
</tr>
<tr>
<td>(7.71, 8.73, 9.36, 10.43)</td>
<td>1.2%</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

Table 4.1: Assembly-weighted model bias and detection uncertainty for all burnup sets in cycles 1 and 2.

Subdivision of the entire burnup range is carried out in such a way in order to extract
detector variations from CASMO/SIMULATE data over a suitable time interval.
Section 4.4 will look at the validity of burnup sets with non-overlapping points being
independent of each other as well as how credible results are of being independent of
burnup subdivision.

Now that BEAVRS data has been overlaid onto SIMULATE data to remove model
bias, all remaining relative errors between BEAVRS data and SIMULATE data for
each assembly over the three burnup divisions can be aggregated as a histogram to
find a 95% confidence level uncertainty. Figure 4-9 plots errors between BEAVRS
data and SIMULATE data for cycle 1, where the histogram frequencies are weighted
by the number of symmetric assembly positions.

From this histogram, it is clear that errors are skewed towards the lower end, with a
few large outliers on the higher end. The RMS value for detection uncertainty in cycle
1 is 0.8%, but taking a more conservative error estimate of 95% confidence yields a
much higher detection uncertainty of 1.6% for cycle 1. Following a similar procedure
for cycle 2 yields a 95% confidence value of 0.9% for detection uncertainty.
Figure 4-9: Histogram of relative error between SIMULATE data and BEAVRS data after correcting for model bias within all assemblies over all burnups in cycle 1. RMS = 0.8%, 95% level = 1.6%.

4.4 Validation of Assumptions for the CASMO/SIMULATE Model

There are two main assumptions that were made when calculating the RMS and 95% confidence values when using the CASMO/SIMULATE model. Firstly, the entire burnup range for both cycles were subdivided into three non-overlapping burnup ranges containing three or four burnups, and it needs to be shown that the results are not dependent on how the subdivisions were made. More specifically, for cycle 1, the entire burnup set (in MWd/kg) is subdivided into the three burnup ranges of (1.02, 1.51, 2.16), (3.30, 4.04, 5.23, 6.52), and (7.61, 8.73, 9.36, 10.43). However, the subdivision could have also been (1.02, 1.51, 2.16, 3.30), (4.04, 5.23, 6.52), and (7.61, 8.73, 9.36, 10.43). Thus, it needs to be shown that detection uncertainty results are independent of the burnup subdivision choice. Table 4.2 shows the results for the 95% confidence interval (CI) of detection uncertainty for all possible burnup subdivisions for both cycle 1 and cycle 2, and the results show that there is very little change in
the results.

<table>
<thead>
<tr>
<th>Cycle 1 Burnup Subdivision</th>
<th>95% CI of Detection Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1.02 1.51 2.16) - (3.30 4.61 6.49 7.51) - (8.70 9.80 11.08 12.34)</td>
<td>1.6%</td>
</tr>
<tr>
<td>(1.02 1.51 2.16 3.30) - (4.61 6.49 7.51) - (8.70 9.80 11.08 12.34)</td>
<td>1.7%</td>
</tr>
<tr>
<td>(1.02 1.51 2.16 3.30) - (4.61 6.49 7.51 8.70) - (9.80 11.08 12.34)</td>
<td>1.6%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cycle 2 Burnup Subdivision</th>
<th>95% CI of Detection Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0.23 1.14 2.11) - (3.20 4.04 5.23 6.52) - (7.71 8.73 9.36 10.43)</td>
<td>0.9%</td>
</tr>
<tr>
<td>(0.23 1.14 2.11 3.20) - (4.04 5.23 6.52) - (7.71 8.73 9.36 10.43)</td>
<td>1.0%</td>
</tr>
<tr>
<td>(0.23 1.14 2.11 3.20) - (4.04 5.23 6.52 7.71) - (8.73 9.36 10.43)</td>
<td>0.9%</td>
</tr>
</tbody>
</table>

Table 4.2: Results of detection uncertainty based on three different ways of subdividing all burnups for each cycle.

The second assumption that needs to be validated that requires a bit more work is to show that non-overlapping burnup subdivisions within the entire burnup set are actually independent of each other. For example, if cycle 1 burnups are divided into the three ranges, (1.02, 1.51, 2.16), (3.30, 4.04, 5.23, 6.52), and (7.61, 8.73, 9.36, 10.43) as before, it needs to be shown that the three burnup ranges are independent of each other. To do this, the results of assembly-weighted detection uncertainty for all adjacent burnup choices of length 3 or 4 are computed after accounting for model bias. If all non-overlapping burnup ranges of length 3 or 4 are truly independent of each other, then the results for detection uncertainty should remain the same regardless of how these burnups are chosen, so long as those burnups are adjacent to each other and represent a short interval for which predictive models are considered accurate. Table 4.3 summarizes the results for detection uncertainty for all possible adjacent burnup choices of length 3 in cycle 1 and 2, while Table 4.4 summarizes the results for burnup choices of length 4 in cycle 1 and 2.

From these two tables, it can be seen that RMS values of detection uncertainty and model bias are roughly consistent for all burnups of length 3 and 4 in cycle 2, where RMS of detection uncertainty ranges from 0.3% to 0.6%. However, within cycle 1,
there are some burnup subsets that have inflated RMS values totaling as much as 1.0%, and these entries are marked in red. In addition, the burnup points common to these high error points are also highlighted in red, and outliers are driving up uncertainty values. With the presence of these outlier burnup points, the errors are much higher than in other cases. With the presence of these outliers, the assumption that the results of non-overlapping burnup sets are independent does not hold true. Recall that these highlighted burnups are the same ones that were found in Section 4.1 to have added model inaccuracies simply due to unstable operating conditions,
further corroborating the existence of outliers at these two points. The simplest way to deal with these outliers is to remove them from the complete burnup range, redo the analysis, and see how the results change. Without these outliers, the detection uncertainties are lower and are also now consistent among all burnup choices for both cycles. The total remaining number of burnup points in the complete range after removing outliers in cycle 1 is now 9, so the burnup range is subdivided into 3 burnup sets of length three. There is no need for another sensitivity analysis based on how to subdivide the entire burnup range as there is now only one way of subdividing the entire burnup range into subsets of length 3.

<table>
<thead>
<tr>
<th>Cycle 1 Burnup Choice</th>
<th>Detection Uncertainty (RMS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.51 2.16 3.30</td>
<td>0.3%</td>
</tr>
<tr>
<td>2.16 3.30 4.61</td>
<td>0.3%</td>
</tr>
<tr>
<td>3.30 4.61 6.49</td>
<td>0.5%</td>
</tr>
<tr>
<td>4.61 6.49 7.51</td>
<td>0.5%</td>
</tr>
<tr>
<td>6.49 7.51 8.70</td>
<td>0.4%</td>
</tr>
<tr>
<td>7.51 8.70 11.08</td>
<td>0.4%</td>
</tr>
<tr>
<td>8.70 11.08 12.34</td>
<td>0.4%</td>
</tr>
</tbody>
</table>

Table 4.6: RMS of detection uncertainty when looking at all combinations of burnup subsets of length 3 in cycle 1 when outliers at 1.02 and 9.80 MWd/kg are removed.

Table 4.5 shows that the 95% CI of detection uncertainty in cycle 1 reduces from 1.6% to 0.8% by running the same CASMO/SIMULATE model without the outlier burnups. Similarly, without the outlier burnups there is now a more consistent level of detection uncertainty across all cycle 1 burnup choices of length three, as shown in Table 4.6. Thus, there is now reason to believe that without these outliers, each
burnup set of length 3 or 4 is independent of each other, as long as the burnups under consideration are adjacent to each other. Cycle 2 does not contain any outlier burnup points, with consistent results among all burnup subdivisions.

### 4.5 Verification of Results with Other Simulation Tools

To show that these results are also not dependent on the model being used, data from MPACT, an alternative neutronics code, is also used as a basis for comparison against BEAVRS data. MPACT is a 3-D full-core transport solver that utilizes the 2-D/1-D method to couple 2-D Method of Characteristics (MOC) solutions radially with lower order 1-D diffusion or $P_3$ solutions axially [21].

For the purposes of comparison, the same methodology used in Sections 4.2 through 4.4 to generate results analogous to those found in Tables 4.5 and 4.6, using MPACT data instead of data from CASMO/SIMULATE. The resulting calculations are shown in Tables 4.7 and 4.8, and there is tremendously close agreement between the final errors after correcting for model bias. Note that only cycle 1 data was available with MPACT.

<table>
<thead>
<tr>
<th>Model</th>
<th>Detection Uncertainty (with outliers)</th>
<th>Detection Uncertainty (without outliers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CASMO/SIMULATE</td>
<td>1.6%</td>
<td>0.8%</td>
</tr>
<tr>
<td>MPACT</td>
<td>1.6%</td>
<td>0.8%</td>
</tr>
</tbody>
</table>

Table 4.7: Cycle 1 95% CI of detection uncertainty with and without outliers at 1.02 and 9.80 MWd/kg using both CASMO/SIMULATE and MPACT.
Table 4.8: RMS of detection uncertainty when looking at all combinations of burnup subsets of length 3 in cycle 1 when outliers at 1.02 and 9.80 MWd/kg are removed in CASMO/SIMULATE and MPACT.

<table>
<thead>
<tr>
<th>Cycle 1 Burnup Choice</th>
<th>Detection Uncertainty in SIMULATE (RMS)</th>
<th>Detection Uncertainty in MPACT (RMS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.51 2.16 3.30</td>
<td>0.3%</td>
<td>0.4%</td>
</tr>
<tr>
<td>2.16 3.30 4.61</td>
<td>0.3%</td>
<td>0.5%</td>
</tr>
<tr>
<td>3.30 4.61 6.49</td>
<td>0.5%</td>
<td>0.3%</td>
</tr>
<tr>
<td>4.61 6.49 7.51</td>
<td>0.5%</td>
<td>0.3%</td>
</tr>
<tr>
<td>6.49 7.51 8.70</td>
<td>0.4%</td>
<td>0.4%</td>
</tr>
<tr>
<td>7.51 8.70 11.08</td>
<td>0.4%</td>
<td>0.4%</td>
</tr>
<tr>
<td>8.70 11.08 12.34</td>
<td>0.4%</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

4.6 Combining Detection Uncertainty and Uncertainty from Using Tilt-Corrected Data

Throughout this chapter, the term detection uncertainty was used to indicate the amount of error that remained from using the CASMO/SIMULATE model after correcting for model bias. Plotting the different values of detection uncertainty across all assemblies and burnup subsets as a histogram similar to Figure 4-9 demonstrates a 95% confidence level for \((\delta_\phi/\phi)_{ij,detection}\) in Equation 3.2. However, this error level does not account for the additional error present due to the fact that tilt-corrected BEAVRS data was used. Equation 3.2 can be used to compute overall time-dependent uncertainty \((\delta_\phi/\phi)_{ij,time-dep}\), and plotting this updated time-dependent uncertainty value for all assemblies in all burnup subdivision as a single histogram yields a 95% confidence value of 1.8% for cycle 1 and 1.9% for cycle 2.

This suggests that if model bias could be completely corrected for, then the resulting time-dependent uncertainty due to fitting data from reactor analysis software to operational data is on the same order as axially integrated measurement uncertainty. The uncertainty that arises from measurement carries over throughout the core burnup and can be used to explain the random fluctuations that occur when trying to fit time-dependent trends to tilt-corrected BEAVRS data.
4.7 Chapter Summary

This chapter details an elaborate process for comparing reaction rates from predictive models to those computed from the detector signals within the BEAVRS benchmark, so a high-level summary of key steps and findings are discussed in this section. The analysis begins with comparing unfiltered SIMULATE data at full power points with tilt-corrected BEAVRS data over short time intervals. This results in findings that data from CASMO/SIMULATE predicts the correct shape of reaction rates over burnup, but is offset from BEAVRS data because of a persistent model bias. Correcting for this bias, the remaining error is coined as detection uncertainty, and plotting these uncertainties for all assemblies over the entire burnup range yields a 95% CI value for detection uncertainty of 1.6% for cycle 1 and 0.9% for cycle 2. However, it is identified that in cycle 1, the assumption that non-overlapping burnup sets are independent of each other is not valid, since outliers at 1.02 and 9.80 MWd/kg drive up the errors for any burnup sets containing these values. Thus, for cycle 1 the analysis for computing the 95% CI for detection uncertainty is repeated without these outliers. The updated results provide an error value that is more in line with values observed from other methods, and the assumption of independent burnup sets holds much stronger.

All analysis for this chapter is then conducted once again, but this time with a different predictive model than CASMO/SIMULATE. Running the tests with the MPACT model indicates that detection uncertainty remains constant across different simulation tools. Finally, Equation 3.2 allows for the calculation of overall time-dependent uncertainty within each assembly for each cycle, and plotting these values as a histogram and finding the 95% confidence value indicates values for both cycles that are consistent with the two methods outlined in Chapter 2. This illustrates the fact that nuclear simulation tools can indeed predict higher-order effects within actual reactor operations. Any discrepancies that arise after correcting for model bias are due to the uncertainty in the underlying BEAVRS data, namely from measurement and post-processing uncertainty.
Chapter 5

Thesis Summary and Conclusions

This research has been inspired by a need for creating error tolerances for future users of the BEAVRS benchmark looking to assess whether discrepancies that arise from formulating new modeling techniques are justified within the uncertainties associated with measurement and processing of operational data. To this end, this work presents a new methodology for uncertainty quantification based on computing time-dependent uncertainty. The results from this procedure are contrasted with methods based on reaction rate map uncertainties, and it is found that all approaches show consistent results and attempt to provide conservative yet realistic uncertainty estimates for the BEAVRS benchmark. Several key assumptions are utilized throughout this thesis in order to arrive at any major conclusions. Section 5.1 will discuss these assumptions, which is then followed by an outline of key results in Section 5.2. Finally, Section 5.3 concludes with future work that could be pursued to strengthen the arguments and claims in this work.

5.1 Primary Assumptions

To understand how results for this work were gathered, a discussion of key assumptions in each section needs to be conducted. Here are four of the main assumptions that should be reiterated.

(1) The Need for a Tilt-Corrected BEAVRS Dataset: Analysis of post-
processed BEAVRS data found that radial reaction rate maps possessed a large tilt in the northwest-southeast corners that resulted in large errors between BEAVRS and Simulation tools, especially at low burnups. While the magnitude of this tilt decreased over burnup, there was still a need to tilt-correct BEAVRS data, since predictive models generate symmetric radial maps for symmetric core loading patterns like the one in BEAVRS. The best-fit plane used to correct for this tilt was assumed to be linear and by removing this tilt, an eighth-core symmetric BEAVRS map could be generated.

(2) **The Use of Predictive Models to Fit Reaction Rates over Burnup:** An important premise for the work in Chapter 4 is that predictive models such as CASMO/SIMULATE and MPACT are valid over a short interval in capturing higher-order effects observed within the reactor, and that measured data should behave in accordance with these models. This motivated work in subdividing entire cycle burnup lengths into smaller subsets to characterize any remaining detection uncertainty observed over short intervals after correcting for model bias. Choosing a burnup set that spanned too long of an interval could cause other physical deviations to come into play that could mask the measurement error.

(3) **Independence of Burnup Sets and Burnup Subdivisions:** While the previous assumption allowed for the calculation of detection uncertainty for short intervals, values for cycle-level detection uncertainty were calculated by assuming that non-overlapping burnup subsets were independent of each other and that errors from the different subsets could be aggregated as a single histogram. Holistic cycle-level errors could now be computed this way, as long as all burnup points within the cycle belonged to a burnup subdivision. To validate this assumption, it was first shown that results were independent of how burnup subdivisions were chosen. It was also demonstrated that detection uncertainties were consistent among all burnup subsets of length 3 or 4, so long as outliers were accounted for.
The Use of a Linear Regression Fit to Model Reaction Rates over Burnup: As a first order approximation, it was assumed in Appendix A that a linear fit could be used to model reaction rate versus burnup. This rests on the theory of the linear reactivity model, and in order to validate this work, conditions for a linear regression model were tested both graphically and statistically. While this worked for certain assemblies within the core, a linear model was not adequate to explain core-wide behavior. Thus, predictive models needed to be used to capture higher-order effects observed within a reactor.

5.2 Key Results and Contributions

This thesis uses a multitude of algorithm and processing steps to quantify time-dependent uncertainty within the BEAVRS benchmark. Here are a few key results from this work.

5.2.1 Proposal of New Uncertainty Quantification Methodology Based on Time Series Analysis

This thesis outlines a novel methodology for computing uncertainty within the BEAVRS benchmark based on time series analysis. Two models are used to compute detection uncertainty, namely the CASMO/SIMULATE model and the linear model. The methodology for the CASMO/SIMULATE model is given in Chapter 4, while work for the linear model is found in Appendix A. Similarly, traditional methods for uncertainty quantification are also presented for comparison. Theoretical analysis of axial uncertainties computes uncertainty using all measurements based on variations of signal strengths by groups. This approach determines uncertainties at each axial point using lookup tables and also sums each axial point and associated uncertainty to calculate axially integrated values. On the other hand, the multiple measurements method computes uncertainty for measurements based on repeated measurements that are conducted by the same detector in the same assembly at a given burnup. The work
for these two methods is found in Chapter 2. For completeness, the 95% confidence values for all traditional UQ methods are shown in Table 5.1, while the 95% confidence estimates of all UQ methods based on time series analysis are presented in 5.2. It should be noted that results from the CASMO/SIMULATE model have been separated into two categories to show how much of the error stems from detection deviation and how much this error level increases after accounting for the uncertainty in using tilt-corrected data. The second column in Table 5.2 indicates the 95% confidence interval of $(\delta_\phi/\phi)_{ij,detection}$ in Equation 3.2, while the third column represents the 95% confidence interval of the cumulative time-dependent uncertainty, $(\delta_\phi/\phi)_{ij,time-dep}$, which accounts for the uncertainty in using tilt-corrected data as well.

### Traditional Methods of Uncertainty Quantification

<table>
<thead>
<tr>
<th>Theoretical Analysis of Axial Uncertainties (Axially Integrated)</th>
<th>Multiple Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle 1</td>
<td>1.4%</td>
</tr>
<tr>
<td>Cycle 2</td>
<td>1.4%</td>
</tr>
</tbody>
</table>

Table 5.1: Summary of results from uncertainty quantification using traditional methods.

### Uncertainty Quantification Methods Based on Time Series Analysis

<table>
<thead>
<tr>
<th>CASMO/SIMULATE Model (before tilt-correction UQ)</th>
<th>CASMO/SIMULATE Model (after tilt-correction UQ)</th>
<th>Linear Regression Model (after tilt-correction UQ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle 1</td>
<td>0.8%</td>
<td>1.8%</td>
</tr>
<tr>
<td>Cycle 2</td>
<td>0.9%</td>
<td>1.9%</td>
</tr>
</tbody>
</table>

Table 5.2: Summary of results from uncertainty quantification using new methods based on time series analysis.

Tables 5.1 and 5.2 show that the uncertainty within the BEAVRS benchmark ranges from 1.4% to 1.8% in cycle 1 and 1.4% to 1.9% in cycle 2. These results indicate that time series analysis methods can be used to model time-dependent behavior.

1The results for the linear regression model can be found in Appendix A.
with measured data behaving in accordance with data from simulation tools. The CASMO/SIMULATE model, for example, predicts reaction rates based on operational conditions, and when accounting for the model bias, the time-dependent uncertainty produces uncertainty results on the same order as methods based on reaction rate map uncertainties. These findings are also independent of type of simulation model used to generate reaction rates. What is more, if uncertainties from using tilt-corrected data could be completely explained, then the remaining detection uncertainty from fitting the CASMO/SIMULATE model to BEAVRS data yield much lower errors than using traditional UQ methods. On the other hand, uncertainty results for the linear model are relatively high and indicate that such simple models cannot explain measured reaction rates over a sustained period of operation.

5.2.2 Quantification of Uncertainty in Using Tilt-Corrected BEAVRS Data

As mentioned in Chapter 3, BEAVRS data contains a significant tilt in the northwest-southeast region at HZP. While the magnitude of this tilt decreases over burnup, the source of this tilt is unknown and was thought to stem from a varying water gap distribution among adjacent assemblies as well as between outer assemblies and the baffle region. This motivated work for quantifying uncertainty in this tilt-correction step, where water gap distribution was varied and optimized in CASMO/SIMULATE to mimic the tilt observed within BEAVRS data. By applying a linear tilt correction to these two data sets, a resulting eighth-core symmetric error map illustrated in Figure 3-8 gives an indication of error in each assembly by assuming a tilt-corrected BEAVRS basis set. Ultimately any time-dependent model utilizing tilt-corrected data incorporates additional uncertainty introduced from tilt-correction using Equation 3.2.
5.2.3 Detection of Outlier Burnup Points

As a consequence of using time-dependent predictive models such as CASMO/SIMULATE, it is found that detection uncertainty remains consistent regardless of the simulation tools being used to predict reaction rates over burnup. Such results bring more credence to using nuclear codes to predict higher order effects observed within actual reactor operations. However, such behavior is also invaluable in detecting outlier burnup points, as shown in Section 4.4. By computing detection uncertainty for each set of adjacent burnup sets, it is observed that inclusion of certain outlier burnup points makes detection uncertainty rise dramatically. These points also happened to be points that suffer from large volatility in power history. Such conditions contribute to additional modeling inaccuracies, and predictive models are unable to capture higher-order reactor effects over short intervals. Calculation of time-dependent detection uncertainty allows for the determination of outlier burnup points that are not at full power and that do not possess stable power histories.

5.3 Future Work

There is still further work that can be conducted to further corroborate the assertions in this thesis. Here are a few avenues for additional investigation.

(1) Reducing Noise in Benchmark Data: The error tolerances computed for BEAVRS can be regarded as still relatively quite high. If future full-core benchmarks are created with hopes of reducing these error tolerances, there should be a push to gather operating data that is less noisy than BEAVRS data. This means having These new benchmarks should look to gain access to more burnup points that are operating at full power and are not plagued with cycle instabilities like that in cycle 1, so that more thorough work on the front of quantifying time-dependent uncertainty with much larger sample sizes can be conducted.

(2) Further Understanding of Causes of Tilt in Operational Data: A key
challenge in the use of time series models has been the existence of the tilt in BEAVRS data, which eventually leads to increased time-dependent uncertainties due to uncertainty in utilizing tilt-corrected data. Future benchmarks should be wary of any pronounced and persistent tilt within the operating data. If such anomalies exist, then there should be a better understanding of the cause of this tilt, so that this phenomenon can be modeled with certainty in simulation tools. This is a significant limitation in work related to optimizing the water gap distribution, where many additional parameters that should have been kept fixed had to be adjusted in order to come up with an explanation for observed data. A better understanding of the source of the tilt will undoubtedly assist in reducing uncertainty generated from imposing any ensuing tilt-correction. Further work could also look at correcting for this tilt by assuming an exponential tilt rather than a linear tilt, to better model the sharp non-linear increases in errors at core peripheries.

(3) **Looking at Higher-Order Regression Models:** Higher-order regression models could fit BEAVRS data much better than assuming a linear fit, but with the use of any such models, however, there should be a rigorous testing of requirements for these regression tools to hold valid. Furthermore, there should also be a scientific basis for introducing higher-order terms that are rooted in explaining the behavior of physical phenomena and not in simply reducing residual error.
Appendix A

Time Dependent Uncertainty in the BEAVRS Benchmark Using A Linear Regression Model

The focus of this chapter is a linear model fit, which is proposed as an alternative but simpler time-dependent model to the CASMO/SIMULATE model. The reason for believing that simple linear fits would work well to explain time-dependent behavior of reaction rates hinges on the principle of the linear reactivity model, which states that at steady-state operations reactivity and hence reaction rates follow a linear trend with burnup [22]. This model is only valid for intervals where the reactor is running at ideal operating conditions with minor disturbances to core power. Thus, the time-dependent analysis for this chapter is once again restricted to looking exclusively at burnup points that are full-power points. Similar to Chapter 4, the analysis will be restricted to using tilt-corrected BEAVRS data. This is because the tilts vary with time and produce additional biases that drive time-dependent data further from behaving linearly. Tests will also be conducted without the outlier points that were detected in Section 4.4 in order to generate comparable results as Chapter 4. Section A.1 presents a mathematical formulation and the requirements for fitting a linear regression to BEAVRS data. Section A.2 tests these requirements, while Section A.3 concludes by discussing the limitations of a linear model and calls for more sophisticated models.
that captures higher-order effects.

## A.1 Formulation of the Linear Model

Models for time series analysis fall under two broad categories - stationary and non-stationary models. Stationary models assume that statistical properties such as mean, variance, and autocorrelation of the underlying distribution do not vary over time, while non-stationary models have statistical properties that are time-dependent.

Written mathematically, a stationary model can be expressed as:

\[ y_t = \mu + \epsilon_t \]  \hspace{1cm} (A.1)

and a non-stationary model can be expressed as:

\[ y_t = \mu_t + \epsilon_t \]  \hspace{1cm} (A.2)

where \( y_t \) is the regressed variable, \( \epsilon_t \) can be viewed as the residual between the regressed and observed value, and \( \mu \) is time-independent, while \( \mu_t \) is time-dependent [23]. For a non-stationary linear regression, \( \mu_t \) can be expressed as:

\[ \mu_t = \beta_0 + \beta_1 t \]  \hspace{1cm} (A.3)

For a linear regression model to be valid, however, it needs to meet four requirements [24]:

1. The linear regression exhibits a high value of \( R^2 \)
2. Residuals of regressed values and measured values are independent of each other with respect to time.
3. Residuals of regressed values and measured values are homoscedastic.
4. Residuals of regressed values and measured values exhibit a normal distribution centered around a 0 mean.
All four of these conditions will be tested in the following section using a combination of visual and statistical techniques.

A.2 Verification of Requirements for a Linear Model

Homoscedasticity refers to the fact that all random variables in the sequence have the same finite variance, while $R^2$ is a measure of goodness of fit of a linear model to the data, and is a value between 0 and 1 that describes the percentage of variable variance that is explained by the linear model. A higher value of $R^2$ implies that a the model is indeed a good fit for the data, and is defined in this case mathematically as [24]:

$$R^2 = 1 - \frac{\sum_T e_t^2}{\sum_T (y_t - \bar{y})^2}$$  \hspace{1cm} (A.4)

where $\bar{y}$ is the mean observed value.

A.2.1 Requirement 1: High $R^2$ values for regressed lines

For each assembly, a linear trendline is fit to the time-dependent tilt-corrected BEAVRS data. When this is done, the $R^2$ value for this fitted model as well as the RMS can be calculated for each assembly. For example, Figure A-1 shows BEAVRS data compared to a linear fit for assembly G9. For this specific assembly, $R^2$ is equal to 95.5% and the RMS is 0.9%. Figures A-2 and A-3 summarize both of these values as radial maps for cycle 1 data and cycle 2 data respectively, where the top number in each assembly corresponds to RMS error, while the bottom number corresponds to the $R^2$ goodness of fit metric. Since the core is eighth-symmetric and numerical results are exactly the same for all symmetric positions, only the results for an eighth-core are shown. These maps illustrate that assemblies with high values of $R^2$ typically have low RMS values.
A.2.2 Requirement 2: Residuals are homoscedastic

As aforementioned, homoscedasticity of residuals refers to the fact that the variance of the residuals approach the same constant value. This means that the variance around the regression line must be roughly the same, and a cone-shaped pattern of data points distributed around the trendline would indicate heteroscedasticity [25]. Visually, a spread level plot of absolute studentized residuals versus regressed values should show the residuals be approximately equally distributed across the range of regressed values without any noticeable patterns [26]. Here, studentized residuals refer to the fact that the residuals have been divided by their standard deviation estimates for normalization purposes. Figure A-4 shows the spread level plot for assembly G9, along with a linear trendline for the data to show how residuals behave as a function of regressed value. A flat trendline demonstrates homoscedasticity.

While visual tests are subject to individual interpretation as to whether residuals are homoscedastic, statistical tests can be used to test for the same criteria. The Breusch-Pagan test, developed by Trevor Breusch and Adrian Pagan and independently suggested by Dennis R. Cook and Sanford Weisberg, tests for the heteroscedasticity in a linear regression model using a test statistic based on the chi-squared distribution [27, 28]. The null hypothesis states that the residuals in the linear regression model
Figure A-2: Cycle 1 RMS (top) and R-Squared (bottom) values based on applying linear model to data set of reaction rate vs. burnup for each assembly. Assembly-weighted total RMS = 0.008.

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
<th>H</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.009</td>
<td>0.008</td>
<td>0.008</td>
<td>0.006</td>
<td>0.009</td>
<td>0.009</td>
<td>0.008</td>
</tr>
<tr>
<td>11</td>
<td>0.008</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.008</td>
<td>0.008</td>
<td>0.006</td>
</tr>
<tr>
<td>12</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
</tr>
<tr>
<td>13</td>
<td>0.008</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
<td>0.005</td>
</tr>
</tbody>
</table>

Figure A-3: Cycle 2 RMS (top) and R-Squared (bottom) values based on applying linear model to data set of reaction rate vs. burnup for each assembly. Assembly-weighted total RMS = 0.010.

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
<th>H</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.017</td>
<td>0.014</td>
<td>0.011</td>
<td>0.010</td>
<td>0.009</td>
<td>0.007</td>
<td>0.010</td>
</tr>
<tr>
<td>11</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>12</td>
<td>0.009</td>
<td>0.007</td>
<td>0.009</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
</tr>
<tr>
<td>13</td>
<td>0.011</td>
<td>0.011</td>
<td>0.011</td>
<td>0.011</td>
<td>0.011</td>
<td>0.011</td>
<td>0.011</td>
</tr>
</tbody>
</table>

80
under consideration are homoscedastic, and if the calculated p-value $p < \alpha$, where $\alpha$ is the statistical significance level, then there is evidence to reject the null hypothesis. For this thesis, $\alpha$ is chosen at a level of 0.05, so a p-value less than this value means that there is a 95% confidence level that the null hypothesis should be rejected. For the case of assembly G9, the calculated p-value is 0.56 so there is little evidence to suggest that the errors are heteroscedastic. A complete list of p-values for the Breusch-Pagan test for each assembly regression is shown in Table A.1. From this table, it can be seen that 25 out of 28 assemblies pass the statistical test, which suggests that errors are homoscedastic for most assembly regressions.

### A.2.3 Requirement 3: Independent residuals with respect to time

Tests for independence of residuals are difficult to visualize, so this section will focus solely on statistical tests to determine whether residuals are correlated to each other. A common avenue for such analysis is to use the Durbin-Watson test for autocorrelation of disturbances [29, 26]. The null hypothesis states that the autocorrelation of the
residuals is 0, implying independence of residuals. The test can be conducted for either positive correlation or negative correlation, so a two-sided test is conducted to test against the alternative hypothesis that the autocorrelation is not equal to 0. Once again, the null hypothesis is rejected for p-values less than 0.05, and Table A.1 indicates that most assemblies pass this test at the 95% level, strongly suggesting that regressed residuals are independent from each other.

A.2.4 Requirement 4: Residuals exhibit a normal distribution centered around 0

Residuals being normally distributed can be shown both graphically and statistically. Visually, a normal Quantile-Quantile (Q-Q) plot can be generated for the residuals to show normality [26]. A Q-Q plot plots studentized residuals against theoretical quantiles of a normal distribution. The plotted points should fall along the line $y = x$, indicating that a specific quantile of residual lies exactly where the expected quantile from a normal distribution is. Figure A-5 shows an example of this for assembly G9, with the red line indicating a best fit line for the plotted data.

![QQ Plot for Assembly G9](image)

Figure A-5: Q-Q plot for linear model applied to for assembly G9 in cycle 1.
Once again, statistical tests can be utilized to test for normality in a more definitive manner. The Shapiro-Wilk test tests the null hypothesis that a sample distribution comes from a normally distributed population [30, 31, 26]. It should be noted that the Shapiro-Wilk test does not assume the underlying sample distribution comes from a standard normal distribution, but instead tests for a general normal distribution with unknown population parameters. A complete list of p-values for each assembly when a linear regression is applied is shown once again in Table A.1. For cycle 1, 27 out of the 28 assemblies resemble a normal distribution.

A.3 Limitations of the Linear Model

In general, analysis of the conditions for a linear regression model indicates that linear models are quite adequate for first-order fitting purposes. Assuming that a linear model is indeed valid and RMS values shown in Figures A-2 and A-3 are indicative of the detection error, \((\delta_\phi/\phi)_{ij,\text{detection}}\) found in Equation 3.2. A similar approach outlined in Section 4.6 can be followed that uses Equation 3.2 to find the 95% value for detection uncertainty. Using the linear model, it is found that the 95% CI for detection uncertainty is 1.9% and 2.0% for cycles 1 and 2 respectively.

While these 95% CI values fit within the same error levels observed in Chapter 2, there are assemblies in both cycles where a linear fit is inadequate, as evidenced by high assembly RMS values as well as cases where multiple statistical tests are rejected in favor of an alternative hypothesis. The primary reason for such behavior is due to the volatile power history for both cycles that call into question the steady-state requirements for linear fitting to be appropriate. Moreover, a linear fit cannot be conducted without knowing the BEAVRS reaction rates a priori, and neglects taking into account any of the actual operating conditions within the reactor. Thus, these limitations necessitate the use of more predictive models that can be used to capture higher-order effects observed within the reactor. Chapter 4 addresses such drawbacks by computing reaction rates from CASMO/SIMULATE to use as bases for comparison against BEAVRS data.
<table>
<thead>
<tr>
<th>Assembly</th>
<th>Breusch-Pagan Test</th>
<th>Durbin-Watson Test</th>
<th>Shapiro-Wilk Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>G9</td>
<td>0.560</td>
<td>0.826</td>
<td>0.885</td>
</tr>
<tr>
<td>G8</td>
<td>0.783</td>
<td>0.630</td>
<td>0.325</td>
</tr>
<tr>
<td>B8</td>
<td>0.341</td>
<td>0.974</td>
<td>0.878</td>
</tr>
<tr>
<td>B9</td>
<td>0.033</td>
<td>0.398</td>
<td>0.488</td>
</tr>
<tr>
<td>E9</td>
<td>0.125</td>
<td>0.094</td>
<td>0.567</td>
</tr>
<tr>
<td>E8</td>
<td>0.089</td>
<td>0.694</td>
<td>0.895</td>
</tr>
<tr>
<td>F10</td>
<td>0.579</td>
<td>0.250</td>
<td>0.372</td>
</tr>
<tr>
<td>D10</td>
<td>0.176</td>
<td>0.458</td>
<td>0.249</td>
</tr>
<tr>
<td>B12</td>
<td>0.217</td>
<td>0.104</td>
<td>0.565</td>
</tr>
<tr>
<td>B13</td>
<td>0.381</td>
<td>0.310</td>
<td>0.240</td>
</tr>
<tr>
<td>B10</td>
<td>0.127</td>
<td>0.186</td>
<td>0.655</td>
</tr>
<tr>
<td>C9</td>
<td>0.954</td>
<td>0.738</td>
<td>0.000</td>
</tr>
<tr>
<td>C8</td>
<td>0.295</td>
<td>0.014</td>
<td>0.201</td>
</tr>
<tr>
<td>F8</td>
<td>0.593</td>
<td>0.460</td>
<td>0.518</td>
</tr>
<tr>
<td>F9</td>
<td>0.178</td>
<td>0.484</td>
<td>0.792</td>
</tr>
<tr>
<td>E11</td>
<td>0.523</td>
<td>0.412</td>
<td>0.933</td>
</tr>
<tr>
<td>E10</td>
<td>0.166</td>
<td>0.274</td>
<td>0.973</td>
</tr>
<tr>
<td>C13</td>
<td>0.043</td>
<td>0.110</td>
<td>0.122</td>
</tr>
<tr>
<td>C12</td>
<td>0.488</td>
<td>0.572</td>
<td>0.259</td>
</tr>
<tr>
<td>C11</td>
<td>0.964</td>
<td>0.044</td>
<td>0.082</td>
</tr>
<tr>
<td>C10</td>
<td>0.429</td>
<td>0.256</td>
<td>0.883</td>
</tr>
<tr>
<td>D12</td>
<td>0.931</td>
<td>0.082</td>
<td>0.419</td>
</tr>
<tr>
<td>A11</td>
<td>0.107</td>
<td>0.780</td>
<td>0.473</td>
</tr>
<tr>
<td>A10</td>
<td>0.057</td>
<td>0.344</td>
<td>0.203</td>
</tr>
<tr>
<td>A9</td>
<td>0.659</td>
<td>0.784</td>
<td>0.167</td>
</tr>
<tr>
<td>A8</td>
<td>0.049</td>
<td>0.102</td>
<td>0.150</td>
</tr>
<tr>
<td>D8</td>
<td>0.760</td>
<td>0.952</td>
<td>0.218</td>
</tr>
<tr>
<td>D9</td>
<td>0.206</td>
<td>0.752</td>
<td>0.906</td>
</tr>
</tbody>
</table>

Table A.1: Summary of p-values from statistical tests that test validity of linear regression model.
Bibliography


