

# Consistent multi-scale uncertainty quantification methodology for multi-physics modelling of prismatic HTGRs

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Thesis accepted in fulfilment of the requirements for the degree  
*Doctor of Philosophy in Nuclear Engineering* at the North-West  
University

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Graduation: October 2020

Student number: 20232608

## **DECLARATION**

I hereby declare that I am the sole author of the dissertation entitled “Consistent Multi-Scale Uncertainty Quantification Methodology for Multiphysics Modeling of Prismatic HTGRs”. All information taken from various journal articles, textbooks or other sources has been referenced accordingly. All collaborative contributions have been indicated and acknowledged.

## ACKNOWLEDGEMENTS

Support of this work was provided between 2014 and 2020 through the U.S. Department of Energy’s funding for Idaho National Laboratory’s contribution to the International Atomic Energy Agency Coordinated Research Project (CRP) on high-temperature gas reactor uncertainties in modeling. This research made extensive use of the resources of the High-Performance Computing Center at Idaho National Laboratory (INL), which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

I would like to thank my promoter Prof. Vishana Naicker for her support and guidance that allowed me to stay focused over the duration of this project.

Dr. Hans Gougar graciously sponsored my involvement in the CRP project and firmly insisted that I finish the doctorate before the next high-temperature gas-cooled reactor is built. His support for this work as co-promotor is gratefully acknowledged.

I owe a special debt of gratitude to Drs. Rike Bostelmann and Pascal Rouxelin. Our manifold discussions guided several pivotal points of this work. Pascal continued his support with various code and model gremlins long after I could fairly expect it from him, despite my untimely interruptions of his *Olympique de Marseille* matches. *Merci beaucoup, Pascal*. Rike tolerated my randomized questions with grace and same-day replies. *Vielen Dank, Rike*.

My inimitable INL colleague Dr. Andrea Alfonsi developed the RAVEN and PHISICS codes. As the resident specialist on RAVEN and uncertainty assessment in general, his advice was critical to the success of the project. *Grazie mille, Andrea!*

Thanks to my parents, who bought our encyclopaedia set when I first started asking “why?” in the 70s, and my sister Liana, who kept a candle burning during some of the darker nights.

Finally, none of this would have happened without Estelle and Sean. She allowed me an obscene amount of time to work on this, and he restrained himself to less than ten interruptions a day, which was impressive for a toddler. Their encouragement, support and love sustained me through the years. *Lief julle*.

*Idaho Falls, October 2020.*

## ABSTRACT

As one of the Generation-IV advanced reactor types, High Temperature Gas-Cooled Reactors (HTGRs) can provide high-quality heat to industrial processes, in addition to saleable and inherently safe power operation. In the United States, several small- and micro-HTGR projects are currently underway, and the assessment of uncertainties in the modelling and simulation of HTGRs is an important aspect of the design and licensing process.

The research reported in this dissertation is focussed on providing a practical example of a statistical uncertainty and sensitivity assessment (U/SA) methodology that can be used by HTGR designers, national nuclear regulators and academic institutions to assess the impact of input uncertainties, across many scales, multiple physics, and time, for several important Figures of Merit (FOMs) such as the core eigenvalue, peak spatial power and maximum fuel temperature. In addition to the quantification of uncertainty in these output parameters, the sensitivity assessment identifies the main contributors to the uncertainties and provides a rationale for future improvements in nuclear data, material property and operational condition uncertainties.

The main objective of this work is the development of a consistent U/SA that can be applied from the lattice to the core spatial domain, and propagation of the non-linear coupled uncertainties that exists between reactor physics and thermal fluid phenomena. The selection of the statistical U/SA approach is motivated by several critical factors unique to HTGRs; the most important being the lack of experimental or operational validation databases and the presence of non-linear phenomena (e.g. coolant bypass flows, graphite thermal conductivity change with irradiation exposure).

The scope of this work includes an assessment of uncertainties in cross-sections, operational boundary conditions and thermal fluid parameters. Two novel contributions include the impact of uncertainties in the core bypass flows on the maximum fuel temperature, and comparisons of the uncertainty and sensitivity results obtained utilizing three energy group structures (2-, 8- and 26 groups).

The proposed methodology is applied to the U/SA of the prismatic modular high-temperature gas-cooled reactor (MHTGR)-350 design, and specifically within the context of the International Atomic Energy Agency (IAEA) Coordinated Research Program (CRP) on HTGR Uncertainty in Modelling (UAM). One of the main contributions of this research is the development of the HTGR UAM benchmark specifications that covers the simulation domain in a phased-approach from the generation of block-level cross-sections to the coupled neutronic/thermal fluid analysis of two important safety case transients (the Control Rod Withdrawal and Pressurised Loss of Cooling events).

The statistical U/SA methodology is successfully implemented and demonstrated using the INL-developed codes PHISICS, RELAP5-3D and RAVEN for the stand-alone and coupled core steady-states and transients, based on perturbed cross-section libraries obtained from the SCALE/Sampler sequence.

Uncertainties in nuclear data (cross-sections and the average number of neutrons produced per fission,  $^{235}\text{U}[\bar{\nu}]$ ) lead to standard deviations (uncertainties of one  $\sigma$ ) of approximately 0.5% in the core eigenvalues of various fresh and mixed MHTGR-350 lattice and core models. For the coupled neutronics/thermal fluid model, local power density uncertainties up to 3.6% were observed in the colder regions of the core, while the local maximum fuel temperature uncertainties reached 1.5% for the models that included thermal fluid uncertainties. The addition of thermal fluid uncertainties dominated the impacts of nuclear data uncertainties in all cases, and it was successfully demonstrated that the statistical methodology propagates the uncertainties from the lattice models to the coupled transients in a consistent manner.

The main contributors to uncertainties in the power density and fuel temperatures during the two transients were uncertainties in the reactor operating conditions (total power, inlet mass flow rate and inlet gas temperature). Variations in the bypass flows did not have significant impact on any of the output variables. For the nuclear data uncertainties it was found that the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  covariance produced the largest sensitivities in terms of its impact on the eigenvalue and peak reactor power. It was also observed that the impact of any nuclear data uncertainties on the maximum fuel temperature was much less significant than the impact on eigenvalue and power.

Another important finding was that although the use of eight or more energy groups is recommended for best-estimate HTGR simulation, two-group models produced acceptable uncertainty and sensitivity results for most FOMs. Since the statistical U/SA methodology is computationally expensive, and most transient solver requirements will scale directly with the number of energy groups, two energy groups could be used by HTGR developers during the early stages of design when larger uncertainty margins can be tolerated.

*Keywords:* HTGR, uncertainty, sensitivity, multiphysics, thermal fluid, cross-section

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## **ABBREVIATIONS AND ACRONYMS**

|        |                                                                 |
|--------|-----------------------------------------------------------------|
| AO     | axial offset                                                    |
| AGREE  | Advanced Gas REactor Evaluator                                  |
| AGR    | advanced gas reactor                                            |
| ANL    | Argonne National Laboratory                                     |
| ART    | Advanced Reactor Technologies                                   |
| BE     | best estimate                                                   |
| BEMUSE | Best Estimate Methods, Uncertainty and Sensitivity Evaluation   |
| BEPU   | best estimate plus uncertainty                                  |
| BISO   | bi-structural isotropic                                         |
| BNL    | Brookhaven National Laboratory                                  |
| BOL    | beginning of life                                               |
| BP     | burnable-poison                                                 |
| BWR    | boiling-water reactor                                           |
| CDF    | cumulative distribution function                                |
| CE     | continuous-energy                                               |
| CENTRM | Continuous ENergy TRansport Model                               |
| CFD    | computational fluid dynamics                                    |
| CFR    | Code of Federal Regulations                                     |
| CR     | control-rod                                                     |
| CRP    | Coordinated Research Program                                    |
| CRW    | control-rod withdrawal                                          |
| DAKOTA | Design Analysis Kit for Optimization and Terascale Applications |
| DBA    | design-basis accident                                           |
| DIN    | Deutsches Institut für Normung                                  |
| DOE    | Department of Energy (United States)                            |
| ENDF   | evaluated nuclear data file                                     |
| EOL    | end of life                                                     |
| FOM    | figure of merit                                                 |
| FZJ    | Forschungszentrum Jülich                                        |
| GA     | General Atomics                                                 |
| GCR    | gas-cooled reactor                                              |

|         |                                                                                |
|---------|--------------------------------------------------------------------------------|
| GFR     | gas fast reactor                                                               |
| GPT     | general perturbation theory                                                    |
| GRS     | Gesellschaft für Anlagen und Reaktorsicherheit                                 |
| GT-MHR  | Gas Turbine Modular Helium Reactor                                             |
| HFP     | hot full power                                                                 |
| HTGR    | high-temperature gas-cooled reactor                                            |
| HTR     | high-temperature reactor                                                       |
| HTTR    | High Temperature Test Reactor                                                  |
| IAEA    | International Atomic Energy Agency                                             |
| INL     | Idaho National Laboratory                                                      |
| INSTANT | Intelligent Nodal and Semi Structured Treatment for Advanced Neutron Transport |
| IPyC    | inner pyrolytic carbon                                                         |
| IRPhEP  | International Handbook of Evaluated Reactor Physics Benchmark Experiments      |
| JAEA    | Japanese Atomic Energy Agency                                                  |
| KAERI   | Korean Atomic Energy Research Institute                                        |
| KI      | Kurchatov Institute                                                            |
| LBP     | lumped burnable poison                                                         |
| LEU     | low-enriched uranium                                                           |
| LFR     | lead-cooled fast reactor                                                       |
| LOFC    | loss of forced cooling                                                         |
| LWR     | light-water reactor                                                            |
| MCNP    | Monte Carlo N-Particle                                                         |
| MFT     | Maximum Fuel Temperature                                                       |
| MG      | multi-group                                                                    |
| MHTGR   | modular high-temperature gas-cooled reactor                                    |
| MRTAU   | Multi Reactor Transmutation Analysis Utility                                   |
| MWt/MWe | megawatt thermal/electrical                                                    |
| NACIE   | NAtural Circulation Experiment                                                 |
| NEA     | Nuclear Energy Agency                                                          |
| NEWT    | New ESC-based Weighting Transport                                              |
| NCSU    | North Carolina State University                                                |
| NNDC    | National Nuclear Data Center                                                   |
| NRC     | Nuclear Regulatory Commission                                                  |
| NSC     | normalised sensitivity coefficient                                             |

|         |                                                               |
|---------|---------------------------------------------------------------|
| OECD    | Organisation for Economic Co-operation and Development        |
| OPyC    | outer pyrolytic carbon                                        |
| ORNL    | Oak Ridge National Laboratory                                 |
| PBMR    | Pebble Bed Modular Reactor                                    |
| PCC     | Pearson correlation coefficient                               |
| PDF     | probability density function                                  |
| PLOFC   | pressurized loss of forced cooling                            |
| PSID    | Preliminary Safety Information Document                       |
| PW      | pointwise                                                     |
| PWR     | pressurized water reactor                                     |
| RCCS    | Reactor Cavity Cooling System                                 |
| RSC     | reserve shutdown control                                      |
| PHISICS | Parallel and Highly Innovative Simulation for INL Code System |
| PIRT    | Phenomena Identification and Ranking Table                    |
| PP      | power peaking                                                 |
| P/R     | PHISICS/RELAP5-3D                                             |
| QA      | quality-assurance                                             |
| RAVEN   | Reactor Analysis and Virtual-control ENvironment              |
| RELAP   | Reactor Excursions and Leak Analysis Program                  |
| ROM     | reduced-order model                                           |
| RPT     | reactivity-equivalent physical transformation                 |
| RPV     | reactor pressure vessel                                       |
| RSC     | reserve shutdown control                                      |
| RSS     | reserve shutdown material                                     |
| SANA    | Selbsttätigen Nachwärmeabfuhr (Secure Decay Heat Removal)     |
| SCALE   | Standardized Computer Analyses for Licensing Evaluation       |
| SCWR    | super-critical water reactor                                  |
| SFR     | sodium fast reactor                                           |
| SNL     | Sandia National Laboratory                                    |
| SUSA    | Software for Uncertainty and Sensitivity Analysis             |
| TF      | thermal fluids                                                |
| TH      | thermal hydraulics                                            |
| THTR    | Thorium High Temperature Reactor                              |
| TINTE   | TIme-dependent Neutronics and TEmpерatures                    |

|        |                                                    |
|--------|----------------------------------------------------|
| TREAT  | Transient Reactor Test                             |
| TRISO  | TRI-structural isotropic                           |
| UAM    | Uncertainty in Analysis and Modeling               |
| U.S.   | United States of America                           |
| U/SA   | uncertainty and sensitivity analysis               |
| V&V    | verification and validation                        |
| VHTR   | very high temperature reactor                      |
| VHTRC  | Very High Temperature Reactor Critical Assembly    |
| VSOP   | Very Superior Old Programs                         |
| VVER   | Vodo-Vodyanoi Energetichesky Reactor               |
| XS     | cross-section                                      |
| XSPROC | Cross (X) Section Processing                       |
| XSUSA  | cross-section uncertainty and sensitivity analysis |

## LIST OF SYMBOLS

| Symbol            | Description                                |
|-------------------|--------------------------------------------|
| $c_p$             | Specific-heat capacity [kJ/kg.K]           |
| $k$               | Thermal conductivity [W/m <sup>2</sup> .K] |
| $k_{eff}$         | Effective multiplication factor            |
| Greek symbols     |                                            |
| $\mu$             | Mean value                                 |
| $\sigma_c$        | Microscopic capture cross-section [barn]   |
| $\sigma_f$        | Microscopic fission cross-section [barn]   |
| $\sigma$          | Standard deviation                         |
| $\nu$             | Average number of neutrons per fission     |
| Chemical formulae |                                            |
| $B_4C$            | Boron carbide                              |
| B                 | Boron                                      |
| C                 | Carbon                                     |
| He                | Helium                                     |
| O                 | Oxygen                                     |
| Pu                | Plutonium                                  |
| Si                | Silicon                                    |
| SiC               | Silicon carbide                            |
| U                 | Uranium                                    |
| $UC_{0.5}O_{1.5}$ | Uranium carbide oxide                      |

## 1. INTRODUCTION

*“Let’s consider your age to begin with — how old are you?”*

*“I’m seven and a half exactly”, Alice said.*

*“You needn’t say ‘exactly’”, the Queen remarked. “I can believe it without that.” Lewis Carroll*

This introduction provides a context for performing uncertainty and sensitivity quantification as part of the high-temperature gas-cooled reactor’s (HTGR’s) design and safety-assessment process. The motivation for this work is driven by the need for a robust uncertainty<sup>1</sup> and sensitivity assessment (U/SA) methodology that can be readily be applied to current and future HTGR designs using existing, established codes. The absence of a significant experimental and operational verification and validation (V&V) basis for HTGRs is an important motivating factor in the consideration of the recommended methodology. The structure of the dissertation is discussed in the final section.

### 1.1 Background and Problem Statement

A significant number of operating nuclear power reactors within the United States of America (U.S.) will reach 60 years of age, and the end of their extended operating licenses, by 2030–2035. In response to this challenge, the U.S. Congress passed the Nuclear Energy Innovation Capabilities Act of 2017, which authorizes the U.S. Department of Energy (DOE) to support the testing and demonstration of advanced reactor concepts and to “. . . enable physical validation of advanced nuclear reactor concepts and generate research and development to improve nascent technologies” (U.S. Congress 2017).

Modular high-temperature gas-cooled reactors (MHTGRs) were identified as one of the six “Generation-IV” advanced reactor concept (OECD/NEA, 2014). The term “advanced reactors”, in this context, does not (necessarily) imply *technically* advanced, but reactor concepts that focus on additional engineered and/or inherent safety principles. Although gas-cooled graphite-moderated reactors have a long history (McCullough 1947), the U.S. Navy’s choice of light-water reactors (LWRs) as the main reactor type for ship propulsion helped to accelerate development of this technology for civilian nuclear energy applications, against which the HTGR could not easily compete. Currently, of the 454 operating nuclear reactors worldwide (IAEA 2019), only one commercial 200 MWe HTGR in China will achieve first criticality in 2020 (Zhang 2016).

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<sup>1</sup> The term “uncertainty” is preferred in this work over “error” because the latter have the connotation of “mistakes” in common usage. The interchangeable use of these two terms is nevertheless observed frequently in literature, especially outside the U/SA domain.

## CHAPTER 1: INTRODUCTION

The design, licensing and operation of any modern nuclear reactor includes the simulation of the reactor's performance at various stages of design maturity and complexity. The software codes developed for reactor analysis need to cover, for example, the mechanical performance and structural integrity of all materials in the system under operating and accident conditions, seismic stability, optimization of thermal-heat generation and transfer, generation of cross-sections and other reactor-physics parameters, and characterization of fission-product releases from the fuel, coolant, and building to determine the eventual worker and public dose rates.

To be effective for the large number of simulations employed in design and safety analyses, the codes need to cover the range of relevant physics using optimized algorithms, exhibit stable and consistent numerical behaviour, and—in a commercial environment—be capable of executing these simulations within short periods of time while achieving acceptable fidelity and accuracy for the stage of design and application. In the domain of primary-system reactor analysis, the large variation in thermal (and, thus, neutronic) properties across the core necessitates the coupled simulation of the neutronic and thermal-hydraulic models to capture all of the physics required to predict challenges to core integrity.

If commercial HTGR operation is the end goal, all these simulation codes require the performance of V&V in compliance with local regulatory standards, such as the provisions of Title 10 Part 50 (U.S. Code of Federal Regulations 1996a) and Part 52 (U.S. Code of Federal Regulations, 1996b) of the U.S. Code of Federal Regulations (CFR).

In general, because no reactor simulation can match the reality of the as-built operating machine with absolute accuracy and infinite precision, and even the measurements of “reality” contain uncertainties, the code V&V process is designed to ensure that the codes predict at least credible and quantifiable “best-estimate” simulation results. This is usually achieved by *validating* the codes' performance against established separate-effects and integral experimental data sets and operational data from similar reactors, if available, in addition to using *verification* code-to-code benchmarks for comparisons with other established or higher-fidelity codes. The assessment of the sources and impact of various model, code and data input uncertainties on important figures of merit (FOMs)—e.g. maximum fuel temperatures and power—therefore forms an integral part of simulation code V&V and drives the need for rigorous uncertainty quantification.

Unfortunately, this task is much harder in the case of the Generation-IV reactors because most, if not all, of the current advanced reactors have very limited validation data sets available. In contrast to the operational data available for LWR/boiling-water reactor (BWR) systems, very few prismatic and pebble-bed HTGRs have ever been built and operated.

Separate-effects and integral experimental data are likewise very limited for HTGRs, and most of the historical data are either not accessible (e.g. protected by commercial or national interests) or incomplete for the purposes of uncertainty quantification (e.g. data listed without measurement uncertainties).

Notwithstanding the significant effort spent so far on best-estimate modeling and simulation of HTGRs in the U.S.<sup>2</sup>, there is currently no example of a comprehensive statistical propagation of HTGR simulation uncertainties across multiple spatial and temporal scales (from lattice cross-section generation to transient core simulations) and multiple physics (neutronics, thermal fluids)<sup>3</sup>. The research reported in this work therefore aims to provide the first example of a robust and consistent method of utilizing existing codes to propagate nuclear uncertainties in HTGR core analysis.

## 1.2 Research Objectives, Contributions and Motivation

The objectives and contributions of this work are summarized as follows:

1. Development of a prismatic HTGR U/SA benchmark based on the MHTGR-350 design that can be used by HTGR core designers, academia and nuclear regulators for verification of their U/SA tools, design-margin characterization, and best-estimate plus uncertainties (BEPU) assessments.
2. Development of a consistent and effective statistical U/SA methodology for the time-dependent neutronic and thermal fluid (multiphysics) analysis of prismatic HTGRs.
3. Application of the methodology using the Standardized Computer Analyses for Licensing Evaluation (SCALE), Parallel and Highly Innovative Simulation for INL Code System/Reactor Excursions and Leak Analysis Program (PHISICS/RELAP5-3D) and Reactor Analysis and Virtual-control Environment (RAVEN) codes to the MHTGR-350 benchmark to establish a set of reference benchmark results, with specific focus on the Phase III coupled steady-state and Phase IV transient exercises.
4. Validation of the SCALE/PHISICS/RAVEN U/SA methodology using measured experimental data from the Very High Temperature Reactor Critical Assembly (VHTRC).

The Phase I–IV benchmark specifications, as summarized in this work, were developed as part of the author’s contributions to the International Atomic Energy Agency (IAEA) Coordinated Research Project (CRP) on HTGR uncertainties in modeling (UAM) between 2012–2020.

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<sup>2</sup> More detail on the current HTGR simulation landscape is provided in Section 2.1

<sup>3</sup> The term “thermal fluids” is preferred in this work as opposed to “thermal hydraulics” to indicate the use of a non-water coolant in HTGRs.

## CHAPTER 1: INTRODUCTION

The selection of the statistical U/SA methodology implemented in this work for HTGRs is motivated by the following considerations:

- The recent advances in general perturbation theory (GPT)-based uncertainty assessments make extensive use of LWR/ boiling-water reactor (BWR) experimental and operational datasets to check and improve the quality of the estimations. This option is not available to the HTGR community due to the very limited quantity of experimental and operational data.
- The non-linear dependencies of some important HTGR thermal fluid parameters cannot currently be treated via the GPT option. An example of this is helium bypass flows between the reflector blocks, which depend on gap sizes caused by swelling and shrinkage of graphite, which in turn depend on fast-fluence exposure and local-temperature history, which themselves depend on bypass flows. Derivation of a first-order perturbation derivative for of all the non-linear coupled parameters in this chain would be extremely challenging, if even possible. One of the secondary contributions of this work is a novel statistical perturbation of helium bypass flow rates to determine impacts on steady-state and transient parameters of interest.
- Even if a global GPT-based approach could be mathematically developed for coupled HTGR neutronic and thermal fluid transient simulations, the source code for commercial or DOE-funded research tools (e.g. STAR-CCM, SCALE, RELAP5-3D, Monte Carlo N-particle [MCNP]) are often not available to all users. The source-code modifications and code-regression testing required for the forward and backward GPT solutions would require significant resources. For this reason, it is not a practical option. Statistical U/SA methods do not require access to the lattice or core-solver source codes.
- General U/SA codes such as SCALE, Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) and RAVEN provide high quality-assurance (QA) standards, a user community and support, low (or no) cost, detailed documentation, and frequent code updates. An HTGR vendor, for example, can therefore complete the implementation of the U/SA method proposed in this work in a shorter time with a higher QA pedigree, as opposed to the “from-scratch” development of a one-off, dedicated HTGR U/SA code.

### 1.3 Dissertation Outline

In Chapter 1, background is provided on the motivation of this work, and the scope and objectives of the research are defined. This is followed in the second chapter by a condensed review of HTGR history and the current status of worldwide projects. A general discussion of the pertinent HTGR physics and state-of-the-art modeling of HTGR systems establishes the context for how Best Estimate plus Uncertainty (BEPU) analysis of HTGRs is used in design and licensing. Chapter 2 also includes an overview of the current status of the IAEA CRP on HTGR uncertainty analysis in modeling (UAM) and the contributions of this research to the CRP. Chapter 3 provides a critical literature review of the latest U/SA methodologies and the justification for selecting a statistical uncertainty-propagation method for HTGR systems.

As a partial validation of the methodology applied on the MHTGR-350 design in Chapters 5–8, the statistical U/SA methodology is applied in Chapter 4 on the experimental VHTRC that preceded the High Temperature Test Reactor (HTTR) design. The uncertainty and sensitivity contributors for two critical core configurations at five temperatures are compared using TSUNAMI and Sampler, PHISICS, and RAVEN.

In Chapter 5, the SCALE, PHISICS, and RAVEN codes are applied to the MHTGR-350 benchmark single block (Exercise I-2a,b) and supercell (Exercise I-2c) models as an application example of the statistical-sampling methodology. The main purpose of these lattice models is the preparation of perturbed cross-sections for the full-core stand-alone neutronics PHISICS/RELAP5-3D (P/R) model utilized in the Sampler and TSUNAMI results for the two Phase II stand-alone neutronics exercises (Chapter 6). This is followed in Chapter 7 by a discussion of the uncertainty and sensitivity results obtained for the thermal fluid stand-alone steady-state (Exercise II-4) and pressurized loss of forced cooling (PLOFC) transient benchmark cases (Exercise IV-1).

The separate and combined impacts of cross-section and thermal fluid uncertainties on the Exercise III-1 coupled steady-state are analysed in Chapter 8. The perturbed 8- and 26-group cross-section data reported in Chapter 5 are used for the generation of several thousand P/R steady-states, and the findings obtained for a series of neutronics-only, thermal fluids-only, and combined steady-states are discussed in detail. Sensitivity indicators are calculated for the eigenvalue, peak power levels, and maximum fuel temperatures in each of these data sets, and the main contributors to the overall uncertainty in these parameters are identified.

## *CHAPTER 1: INTRODUCTION*

The propagation of the separate and combined cross-section and thermal fluid uncertainties is concluded in Chapter 8 by utilizing the coupled P/R steady-states generated during Phase III as the starting points for the control-rod withdrawal (CRW) transient defined for Exercise IV-2 and to illustrate how the proposed methodology can be utilized for a typical HTGR safety case. The main findings and conclusions of the study are summarized in Chapter 9, which also includes recommendations for areas of further study.

Appendix A contains additional information on the Organisation for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA) MHTGR-350 benchmark, and Appendix B provides a description of the software codes used in this work (i.e. SCALE, PHISICS, RELAP5-3D, and RAVEN). A listing of the author's journal and conference publications related to this work is provided in Appendix C while data that could be of use to other benchmark participants are included in Appendix D.

## 2. HTGR DEVELOPMENT AND SIMULATION

*“Essentially, all models are wrong, but some are useful.” George E.P. Box*

This chapter starts with a short historical summary of the development and commercialization of HTGRs<sup>4</sup>. This is followed by a discussion of the most-important physics and thermal fluid characteristics of modern HTGRs, which leads to the requirements for the generation of cross-sections for HTGR core calculations.

### 2.1 History and Current Status of HTGRs

Following the success of the first graphite pile developed by Enrico Fermi’s team in 1942 (Argonne National Laboratory (ANL) 2019), the Power Pile Division of Clinton Laboratories (later the Oak Ridge National Laboratory [ORNL]) decided in 1946 that an engineering team would be created to design a steam cycle, helium-cooled, high-temperature pile using beryllium oxide as moderator to obtain a thermal spectrum (McCullough et al. 1947). The design was based on a patent by Farrington Daniels filed in 1945 (Daniels 1957); he proposed a gas-cooled pebble bed, with an outlet temperature of up to 2,000°C. Although these early high-temperature reactor proposals were early companions of the first LWRs, the large-scale deployment of HTGRs never materialized, and only a few commercial and research facilities have so far been operated (Table 2-1).

The Dragon Reactor Experiment reactor—which operated successfully between 1964 and 1975—had a thermal output of 20 MW, achieved a gas outlet temperature of 750°C, and was used for irradiation testing of fuels and components utilized in later designs (e.g. the Thorium High Temperature Reactor (THTR) in Germany and the Fort St. Vrain power plant in Colorado, U.S.). The advanced gas reactors (AGRs) are CO<sub>2</sub>-cooled graphite-moderated designs, and although the typical AGR outlet gas temperature of 650°C is not much lower than HTGRs, this reactor type is usually not seen as part of the HTGR family because AGRs use a clad fuel rod similar to pressurized water reactors (PWRs).

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<sup>4</sup> Clarification on the use of “HTGR” in this work: several terms have been used to describe reactor designs with outlet temperatures substantially higher than LWRs. Gas-cooled and molten-salt-cooled high temperature reactors are both part of the HTR class, and within the HTGR class the terms *very high temperature reactor* (VHTR) and *modular* HTGR have been used since the early 1990s. VHTRs typically have helium outlet temperatures in excess of ~750°C, which creates additional demands on the development of high-temperature materials. “MHTGR” is used in the context of a relatively small HTGR “unit”, in the 100–400 MWt range, which could be scaled to deliver combined “packs” of 2, 4, 6, or more units on a power utility site. A few “traditional” high-output (>0.7–3.5 GW) single-facility HTGR designs were proposed and operated in Germany and the U.S., but this approach has not been pursued in the last 30 years due to the (claimed) improved safety and economic business case of modular HTGRs.

## CHAPTER 2: HTGR DEVELOPMENT AND SIMULATION

The development of the two main HTGR types—characterized by their low-enriched uranium (LEU) pebble or prismatic-block fuel forms—occurred mainly in Germany (pebble beds) and the U.S. (prismatic). The German interest in pebble-bed HTGRs started in the late 1950s when Rudolf Schulten refined the Daniels pile concept by designing a fuel pebble that contains thousands of coated UO<sub>2</sub> fuel-kernel particles, and surrounding it with a layer of SiC between two layers of pyrolytic carbon (Figure 2-1). This tristructural isotropic (TRISO) fuel form was used in almost all subsequent pebble-bed and prismatic HTGR designs as the main safety argument and primary barrier to fission-product releases.

Table 2-1. Operational HTGRs.<sup>5</sup>

| Description and Location                              | Type and Power Rating (MWt) | Operational Period and Status    |
|-------------------------------------------------------|-----------------------------|----------------------------------|
| Dragon, UK                                            | Prismatic, 20 MWt           | 1964-1975. Decommissioned.       |
| Peach Bottom 1, USA                                   | Prismatic, 115 MWt          | 1966-1974. Decommissioned.       |
| Arbeitsgemeinschaft<br>Versuchsreaktor (AVR), Germany | Pebble bed, 46 MWt          | 1967-1988. Being decommissioned. |
| Fort St Vrain, USA                                    | Prismatic, 842 MWt          | 1979-1989. Decommissioned.       |
| THTR, Germany                                         | Pebble bed, 750 MWt         | 1983-1989. Decommissioned.       |
| HTTR, Japan                                           | Prismatic, 30 MWt           | 1998-current. Operational.       |
| HTR-10, China                                         | Pebble bed, 10 MWt          | 2000-current. Operational.       |

Japan and the U.S. have primarily pursued the prismatic HTGR designs. The interest in prismatic HTGRs in Japan dates to 1975 with the development of the Semi-Homogeneous Experiment, which was converted into the VHTRC in 1986 (Terry et al. 2004). This eventually led to the construction and very successful operation of the 30 MW HTTR in 1998 (IAEA 2003), which is the only prismatic HTGR currently still operable in shutdown after Fukushima. In the U.S., the prismatic Peach Bottom 1 unit was the first prototype HTGR, and it operated successfully for 7 years between 1967 and 1974 (Terry et al. 2004). It provided valuable confirmations of reactor physics and design methods, as well as an operational database for the helium-purification system and steam-generator tube materials. The engineering and development experience built up during the Peach Bottom project led to the commissioning of the 842 MWt Fort St. Vrain in Colorado in 1976 (Brown et al. 1987).

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<sup>5</sup> The AGRs in the United Kingdom are excluded from this list because the operational temperature, coolant and fuel design differ significantly from HTGR designs. Data from the AGRs can therefore not be used directly for HTGR validation purposes, except for nuclear graphite materials research.

## CHAPTER 2: HTGR DEVELOPMENT AND SIMULATION

This commercial facility was the first HTGR demonstration power plant by the U.S. DOE, but it experienced low availability due to issues with the helium-circulator design that utilized water-lubricated bearings. It is nevertheless seen as a successful demonstration and test bed for the performance of several important HTGR technology aspects, e.g. the block-based TRISO fuel form, fuel handling, and reactor internals systems (Brey 2003).

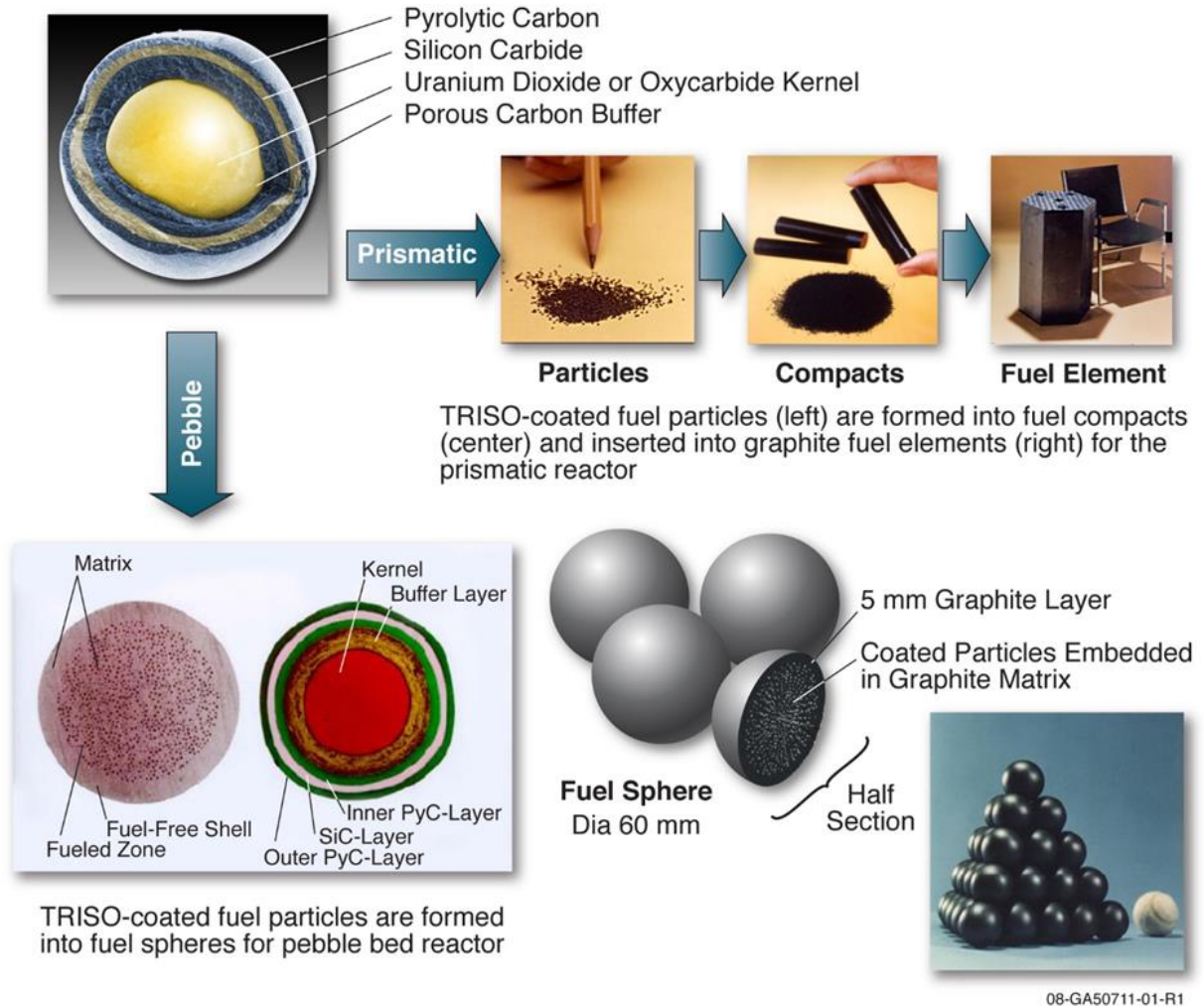


Figure 2-1. HTGR fuel forms: TRISO fuel particles consolidated into a graphite matrix as prismatic blocks (upper right) or pebbles (lower right). (Allen et al. 2010).

The 350 MWt General Atomics MHTGR design—an annular core and a simplified version of the MHTGR-350 design developed in the mid-80s (Bechtel 1986)—is used in this study as the basis for the prismatic HTGR design specified for the IAEA CRP on HTGR UAM Phase I (Strydom & Bostelmann 2017) and Phase II (Rouxelin & Strydom 2017; Strydom 2018). An overview of the MHTGR-350 design is provided in Appendix A.

Current examples of commercial projects in the U.S. include the X-Energy 200 MWt pebble-bed modular HTGR (Power 2018) and the Framatome 625 MWt steam cycle (SC)-HTGR (Lommers et al. 2013). The Canadian-based STARCORE company developed a small 50 MWt prismatic HTGR that targets remote oil-sands and military sites (Short et al. 2016), and a U.S. study on advanced test and demonstration reactors (Petti et al. 2017) included an INL-designed 200 MWt prismatic HTGR test reactor capable of testing various coolants and materials in separated pressurized loops.

## 2.2 The Modeling and Simulation of HTGRs

The main characteristics of HTGR designs are a low power density ( $\sim 3\text{-}6\text{ W/cm}^3$ ), moderation by a very robust solid-graphite ceramic with a large thermal-heat capacity and inertia, cooled by a single-phase gas that is transparent to neutrons, and a TRISO ceramic fuel form that can tolerate very high temperatures sustained over days during a complete loss of cooling. The modular HTGR core designs are also typically tall and thin to enhance passive heat transfer from the core in the event of a loss of forced circulation.

Although both HTGRs and LWRs are thermal reactor systems, HTGRs require additional consideration to capture the double heterogeneous nature of the dispersed TRISO fuel in a graphite matrix. The treatment of both neutron scattering and resonance capture in graphite are complex and not adequately captured using the methods traditionally used in LWRs. For transient analysis, Doppler temperature feedback acts on the individual TRISO fuel particles, but full-core models cannot resolve phenomena at this scale without a suitable weighted averaging over space and energy. For burnup calculations, the second (fuel-compact) level of heterogeneity must also be resolved to capture the local effects of burnable poisons while accurately propagating the flux-suppression effects through and between blocks.

### 2.2.1 Nuclear Cross-sections and Covariances

Regardless of reactor type or application, basic nuclear data are required that characterize the interaction of neutrons with various nuclides of interest as a function of energy and multiple reaction types (absorption, fission, scattering etc.). In the U.S., experimental nuclear data results are evaluated by nuclear data organisations that review multiple measurements and agree on the highest-quality measurements before publishing the data as evaluated nuclear-data files (ENDFs). The ENDFs usually consist of a mixture of high-fidelity measured data at internationally accredited laboratories (e.g. Brookhaven National Laboratory [BNL]), lower-fidelity measurements of specific nuclides, and theoretical models of unresolved resonance regions.

The creation of an ENDF starts with the collection of experimental data. An evaluation is then created by combining the experimental data with nuclear-model predictions and fitting functions and the results are tabulated into an evaluated nuclear data set.

## CHAPTER 2: HTGR DEVELOPMENT AND SIMULATION

The use of nuclear models is necessary to fill in the gaps where experimental results do not exist (McEwan 2013). Several organisations collect and publish these data sets. In the U.S. and Canada, the Cross-Section Evaluation Working Group of the National Nuclear Data Center produces the ENDF/B files while the Joint Evaluated Fission and Fusion File (JEFF) organisation comprises members of the OECD NEA. They produce the JEFF database, which is also in the ENDF format. The Japanese Nuclear Data Committee handles the Japanese Evaluated Nuclear Data Library. This effort is coordinated through the Nuclear Data Center at the Japan Atomic Energy Agency (JAEA).

The work reported in this dissertation will use data libraries included in Release 6.2 of SCALE, which utilizes the ENDF/B-VII.1 library (Chadwick et al. 2011), in addition to other data sources. (The latest ENDF/B-VIII.0 library [Brown et al. 2018] will be used with the next release of SCALE 6.3 in 2020). SCALE includes both multigroup (MG) and pointwise (PW) continuous-energy (CE) nuclear data libraries, which were processed using the AMPX code system. The CE libraries are used for Monte Carlo calculations with CE-KENO and are also used by the PW discrete ordinates code Continuous ENergy TRansport Model (CENTRM) to obtain PW flux spectra for computing self-shielded MG cross-sections. This sequence is especially important for double heterogeneous systems, where the only limitation currently inherent in the SCALE approach is the use of a typical PWR base-weighting function instead of a dedicated HTGR spectrum (see the SCALE User Manual Section 10.1.2.1 for more detail) (Rearden et al. 2016). All KENO-VI and New ESC-based Weighting Transport (NEWT) MG results reported in this work utilized the 252-MG libraries that were released with Version 6.2 of SCALE. One of the improvements made from the older 238-MG library is the extension of the thermal-energy range where upscattering reactions are included from 3 to 5 eV—a change that is especially beneficial for graphite-moderated HTGR systems.

Figure 2-2 shows an example of changes made to the  $^{238}\text{U}(n,\gamma)$  cross-section for the ENDF/B-VII.1 and the new ENDF/B-VIII.0 libraries (National Nuclear Data Center (NNDC) 2019). The plot shows the differences as the ratio of the ENDF/B-VII.1 data to the ENDF/B-VIII.0 data. The significant differences between the two libraries in the resolved and unresolved resonance regions can clearly be seen in this plot. In addition to detailed cross-section data, covariance information is also provided for a subset of the available nuclides. Covariances provide information on correlations between measured cross-sections that will always have experimental uncertainties associated with them.

Following the derivation presented by Dunn (2000), the ENDF value provided for each cross-section represents an estimate  $\langle x \rangle$  of the true cross-section value  $x$ . (Here  $x$  could be the fission cross-section for  $^{235}\text{U}$ , for example). If  $f(x)$  is defined as the density function that represents the variation associated with the measured cross-section data, the estimate  $\langle x \rangle$  represents the first moment of the density function and is defined as

$$\langle x \rangle = \int x f(x) dx \quad (2-1)$$

where

$$\int f(x) dx = 1 \quad (2-2)$$

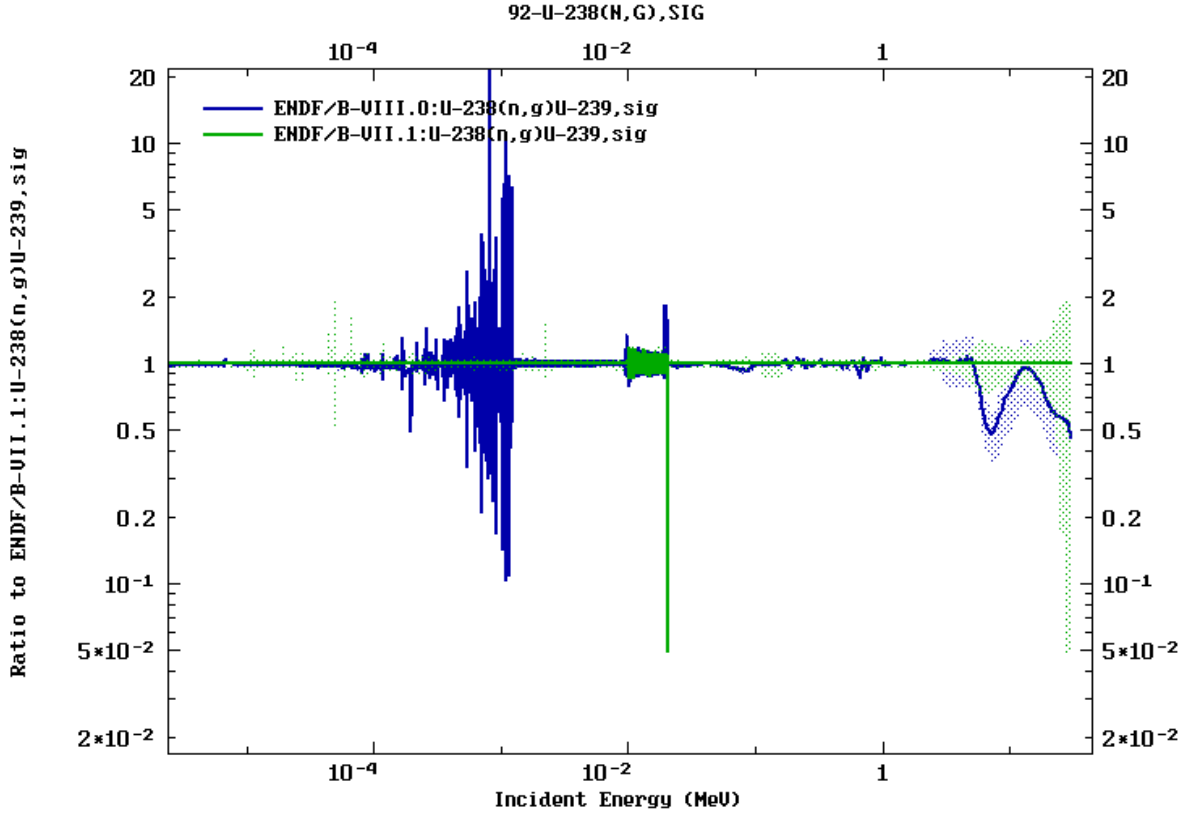


Figure 2-2. Comparison of  $^{238}\text{U}$  (n,γ) cross-section: ratio of ENDF/B-VII.1 (green) to ENDF/B-VIII.0 (blue).

The difference between the true value of  $x$  and the estimate  $\langle x \rangle$  is the deviation  $\delta x$ , defined as

$$\delta x = x - \langle x \rangle \quad (2-3)$$

Using similar definitions for a second cross-section quantity  $y$ ,  $\langle y \rangle$  and  $\delta y$ , the second moment of the density function  $f(x,y)$ , or the covariance of  $x$  with  $y$ , can then be defined as

$$\text{COV}(x, y) = \langle \delta x \delta y \rangle = \iint (x - \langle x \rangle)(y - \langle y \rangle) f(x, y) dx dy \quad (2-4)$$

The covariance of  $x$  with  $y$  (e.g. the covariance of the  $^{235}\text{U}$  fission cross-section with the  $^{235}\text{U}$  (n,γ) cross-section) appears as the off-diagonal terms in the  $^{235}\text{U}(n,f), ^{235}\text{U}(n,\gamma)$  covariance matrix.

## CHAPTER 2: HTGR DEVELOPMENT AND SIMULATION

The covariance of  $x$  with itself is known as the variance and forms the diagonal of the covariance matrix. It is defined as

$$VAR(x) = \langle \delta x^2 \rangle = \int (x - \langle x \rangle)^2 f(x) dx \quad (2-5)$$

The standard deviation, or uncertainty, in  $x$  is obtained by taking the square root of the variance:

$$STD.DEV(x) = \sigma(x) = \sqrt{VAR(x)} = \sqrt{\langle \delta x^2 \rangle} \quad (2-6)$$

The correlation coefficient  $\rho(x, y)$  between  $x$  and  $y$  can finally then be defined in terms of the covariance and standard deviation

$$\rho(x, y) = \frac{COV(x, y)}{\sigma(x)\sigma(y)} \quad (2-7)$$

In practice, the ENDF data consist of relative quantities of interest, as opposed to the absolute formulations shown above. The relative covariance, relative variance, and relative standard deviation are defined as

$$RCOV(x, y) = \frac{COV(x, y)}{\langle x \rangle \langle y \rangle} \quad (2-8)$$

$$RVAR(x) = \frac{VAR(x)}{\langle x \rangle \langle x \rangle} \quad (2-9)$$

$$R\sigma(x) = \frac{\sigma(x)}{\langle x \rangle} \quad (2-10)$$

An example of the ENDF/B-VII.1  $^{238}\text{U}$  (n,  $\gamma$ ) covariance matrix is shown in Figure 2-3. In the case of SCALE 6.2, the 56- and 252-group covariance libraries are based on available ENDF/B-VII.11 data for 187 nuclides, combined with the previous SCALE 6.1 covariance data retained for the ~215 nuclides not available in ENDF/B-VII.1. It is important to note that the SCALE covariance libraries are different from the standard covariance libraries released with ENDF/B-VII.1. The SCALE covariance library is based on several different uncertainty approximations with varying degrees of fidelity relative to the actual nuclear data evaluation. The library includes high-fidelity evaluated covariances obtained from ENDF/B-VII.1, and ENDF/B-VI whenever available, and is augmented by low-fidelity covariances that are based on results from a collaborative project funded by the U.S. DOE Nuclear Criticality Safety Program. More detail on the cross-section and covariance data used in SCALE 6.2 can be found in Section 10 of the User Manual (Rearden et al. 2018).

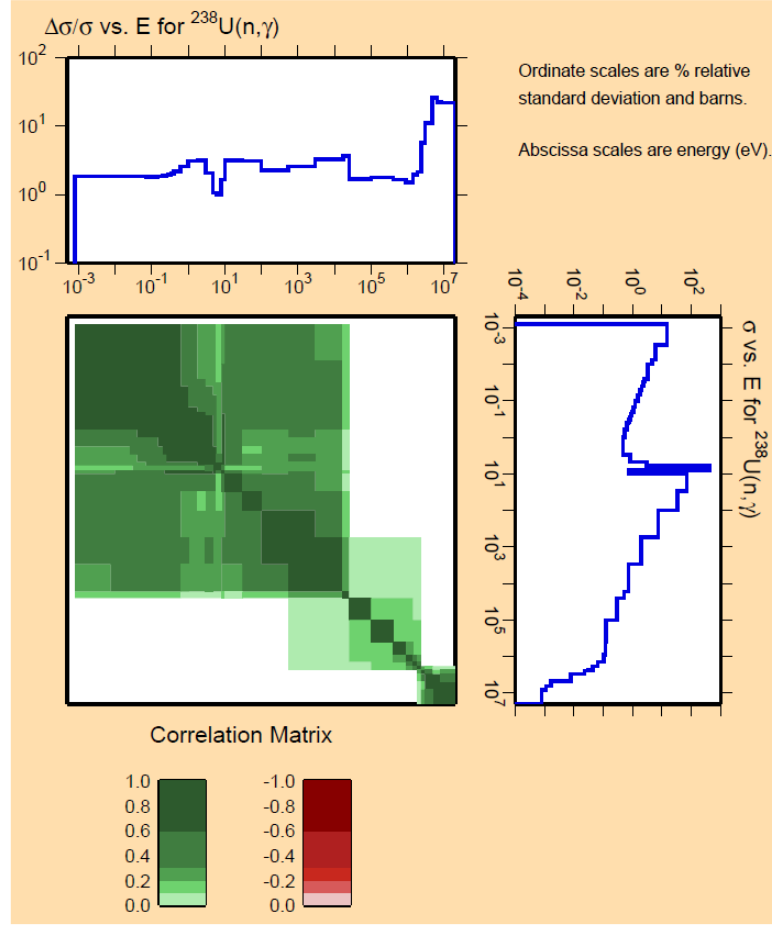


Figure 2-3. ENDF/B-VII.1  $^{238}\text{U}$  (n,γ) covariance matrix (NNDC, 2019).

## 2.2.2 HTGR Lattice Neutronics and Energy Group Structures

Neutronics analysis of LWRs typically uses a two-step approach that starts with a neutron-transport computation at the fuel-pin or assembly level. The fine-energy group and detailed spatial results are obtained from either Monte Carlo or deterministic transport solutions of an infinitely reflected lattice cell using one of the ENDF libraries described in Section 2.2.1. Subsequent to the self-shielding cell calculation, the fine-energy group structure is collapsed into a more manageable number of groups. The resulting coarse (or few) energy-group data can be tabulated as a function of fuel temperature or water density for use in full-core calculations, as is often done for large-scale transient models. This process is well-established and usually involves a trade-off between accuracy and computational efficiency if a larger number of coarse groups is desired.

In contrast to the LWR case, an “assembly” is not defined for pebble-bed HTGRs, and even if a geometrical unit, such as the fuel block, could be identified for prismatic HTGRs, the HTGR assemblies are spatially much more strongly coupled than in the LWR domain.

A two-step approach can lead to significant errors for LEU-fueled cores with strong  $^{238}\text{U}$  neutron-absorption resonances, a graphite moderator and a “thin” annular core design (Ortensi 2012), as is the case for the MHTGR-350 design. The “true” size of HTGR “assemblies”—from the viewpoint of a fast neutron—is therefore significantly smaller than the physical size of a single fuel block (Table 2-2). For a fast neutron born in an LWR spectrum, the apparent size of the core is 10 times larger (300 mfps) than is an HTGR core (Ougouag et al. 2018). A comparison between the neutron spectra of two water-cooled systems (PWR and SCWR), three fast reactor systems (SFR, LFR and GFR), and the VHTR is shown in Figure 2-4.

There are multiple levels of heterogeneity in HTGR cores: the TRISO fuel particles embedded in the graphite matrix of the fuel compacts, the fuel compacts within the fuel blocks, and the fuel blocks within the core surrounded by a large reflector region (Figure 2-1).

Table 2-2. Comparison of HTGR and LWR nuclear characteristics (Baxter, 2010).

| Description                                           | HTGR | LWR    |
|-------------------------------------------------------|------|--------|
| Core average power density ( $\text{W}/\text{cm}^3$ ) | 3–7  | 50–105 |
| Diffusion coefficient (cm)                            | 0.86 | 0.16   |
| Neutron mean free path (cm)                           | 3–4  | 8–15   |
| Diffusion length (cm)                                 | 54.0 | 2.8    |
| Migration length (cm)                                 | 57   | 6      |

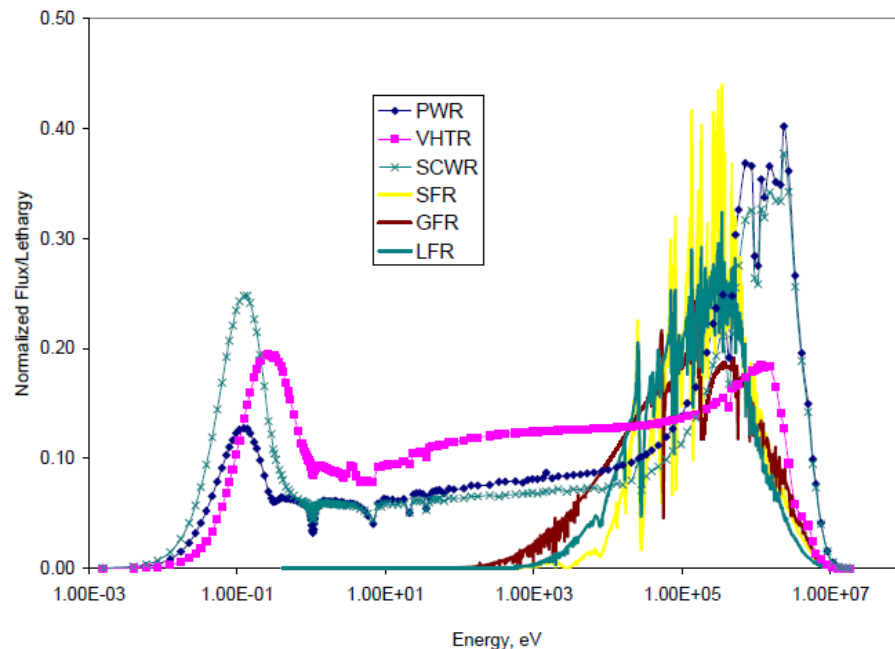


Figure 2-4. Comparison of Generation-IV neutron energy spectra (Taiwo & Hill 2005).

Features that typically require non-diffusion (transport) solutions include the strong spatial absorbers such as the control rods in the reflector and large void regions, where neutron streaming is significant (e.g. control-rod channels, the void above the core). The presence of coated burnable-poison particles in the corners of prismatic fuel blocks (the green dots in Figure 2-5) adds additional complexities during the preparation of proper self-shielded cross-sections, and is especially important for depletion sequences (Rouxelin 2019; Sihlangu et al. 2019).

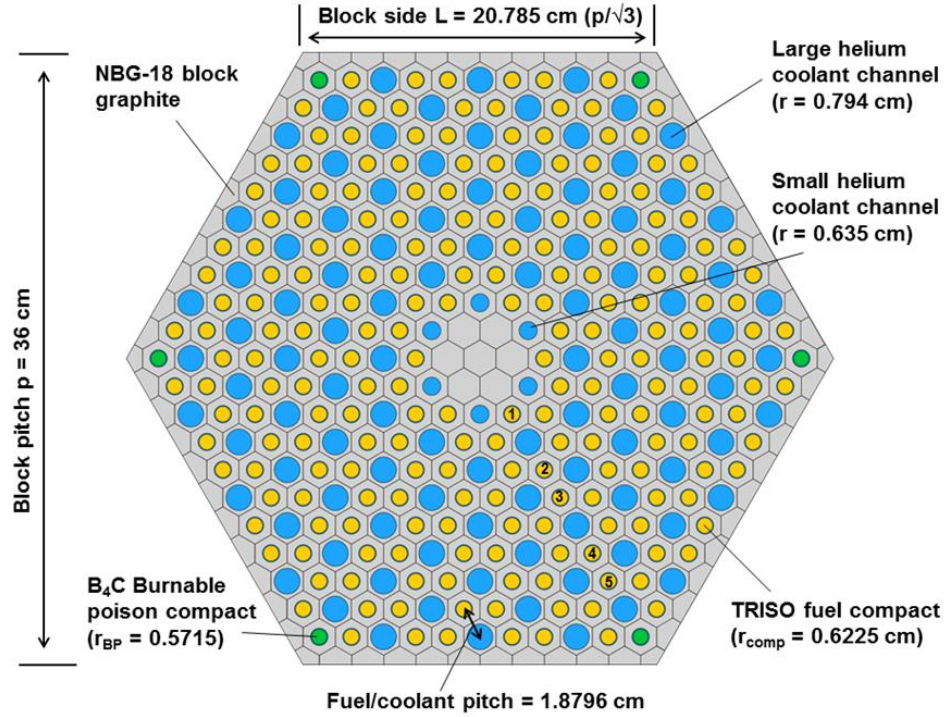


Figure 2-5. MHTGR-350 fuel block.

The impact of the issues indicated above can be treated partially by using a larger number of energy groups for the core solution by capturing the environmental spectral effects more accurately, but for most transient simulations, the use of more energy groups also requires more computational resources.

The choice of the few-group energy structure is a significant user choice that impacts core calculations and is an example of an epistemic uncertainty factor that can be reduced for HTGR simulations with further research. Although the effects of HTGR energy-group-structure selection for core simulations has been investigated for *nominal* calculations (e.g. Gougar 2018, Han et al. 2008, and Zhang et al. 2011), the impact of this factor has not been determined in the presence of other input uncertainties.

## CHAPTER 2: HTGR DEVELOPMENT AND SIMULATION

Rouxelin (2019) most recently developed a statistical sampling and response surface approach from the very fine lattice library to determine optimal group boundaries for HTGR core simulation. His SCALE/PHISICS/RAVEN sequence could be a valuable tool to minimize the uncertainties related to the choice of few-group structures for HTGR simulations.

The upper energy-group boundaries are shown in Table 2-3 for six options, varying between 6 and 26 groups. The thermal boundary for all but one of these structures is 2.38 eV (shown in bold font). It was found that the General Atomics (GA) nine-group Fort St. Vrain structure does not perform as well as the 8-group structure proposed by Han (2008) because the older GA cores were fueled with a mixture of highly enriched uranium and fertile thorium, and the nine-group library was optimized for Th-fueled systems. Han's study also concluded that the 26-group structure developed at Forschungszentrum Julich (FZJ) for HTGR analysis (IAEA 2003) produces the best eigenvalue and power-density results, as compared with a reference CE Monte Carlo transport solution.

For this dissertation research, an 8-group structure was selected to provide a reasonable trade-off between accuracy and transient-calculation cost. Because the SCALE 252 fine group energy boundaries are not located exactly at Han's suggested 8-group boundaries, an 8-group SCALE structure was chosen by selecting the closest available energy boundaries. The lattice cases reported in Chapter 5 have also been repeated with the FZJ 26-group structure to assess the impact of this choice on the FOM uncertainties, in addition to utilizing all 252 groups for the VHTRC comparisons in Chapter 4. For the CRW transient discussed in Chapter 8, a 2-group structure was also included to determine whether such a low number of energy groups could still provide useful uncertainty and sensitivity information.

It should be stressed that the main aim of this work is not to determine the best nominal values that can be achieved, but rather an assessment of uncertainties inherent in HTGR-physics simulations and, specifically, the impact of uncertainties in cross-section data on the Phase III and IV power-density and fuel-temperature outputs.

Table 2-3. Six examples of HTGR energy-group structures (upper energy boundaries shown in eV).

| Group Number | FZJ (26g) | TREAT & HTTR (10g) | Fort St. Vrain (9g) | Han (8g) | Selected SCALE boundaries (8g) |
|--------------|-----------|--------------------|---------------------|----------|--------------------------------|
| 1            | 2.00E+07  | 4.00E+07           | 2.00+07             | 2.00E+07 | 2.00E+07                       |
| 2            | 7.90E+06  |                    |                     |          |                                |
| 3            | 3.68E+06  |                    |                     |          |                                |

*CHAPTER 2: HTGR DEVELOPMENT AND SIMULATION*

| Group Number | FZJ (26g)    | TREAT & HTTR (10g) | Fort St. Vrain (9g) | Han (8g)     | Selected SCALE boundaries (8g) |
|--------------|--------------|--------------------|---------------------|--------------|--------------------------------|
| 4            | 6.39E+06     |                    |                     |              |                                |
| 5            | 1.11E+05     | 1.16E+05           | 1.83E+05            | 1.83E+05     | 2.00E+05                       |
| 6            | 1.93E+04     |                    |                     | 9.12E+03     | 9.50E+03                       |
| 7            | 3.36E+03     | 3.48E+03           |                     | 2.04E+03     | 2.20E+03                       |
| 8            | 1.59E+03     |                    |                     |              |                                |
| 9            | 749          |                    | 961                 |              |                                |
| 10           | 275          |                    |                     |              |                                |
| 11           | 130          |                    |                     |              |                                |
| 12           | 61           |                    |                     |              |                                |
| 13           | 29           |                    |                     |              |                                |
| 14           | 14           |                    |                     |              |                                |
| 15           | 8.320        | 8.100              | 18                  |              |                                |
| 16           | 5.040        |                    | 3.930               |              |                                |
| 17           | <b>2.380</b> |                    | <b>2.380</b>        | <b>2.380</b> |                                |
| 18           | 1.290        |                    |                     |              |                                |
| 19           | 0.650        | 0.625              | 1.600               | 1.590        |                                |
| 20           | 0.350        |                    |                     |              |                                |
| 21           | 0.200        | 0.209              | 0.420               | 0.430        | 0.450                          |
| 22           | 0.120        |                    |                     |              |                                |
| 23           | 0.080        | 0.076              | 0.100               | 0.120        | 0.125                          |
| 24           | 0.050        | 0.047              |                     |              |                                |
| 25           | 0.020        | 0.020              | 0.040               |              |                                |
| 26           | 0.010        |                    |                     |              |                                |

### 2.2.3 HTGR Thermal Fluids

The assessment of multiphysics uncertainties reported in Chapters 7 and 8 utilizes a progression of exercises to characterize the impact of thermal fluid input uncertainties. Phenomena for gas-cooled reactors were addressed in detail during the development of several Phenomena Identification and Ranking Tables (PIRTs) summaries prepared for the U.S. Nuclear Regulatory Commission (NRC, U.S. NRC 2008, U.S. NRC 2019). Seven aspects of HTGR simulation were identified that require specific attention due to their importance and relatively low knowledge level: core coolant-bypass flows, power/flux profiles, outlet-plenum flows, reactivity-temperature feedback coefficients, vessel and reactor-cavity cooling system emissivity, reactor-vessel-cavity air circulation and heat transfer, and convection/radiation heating of the upper vessel. The NRC is currently most interested (from a safety point of view) in PLOFC and depressurized loss of forced cooling (DLOFC) events, as well as the reactivity insertion via a CRW.

Input uncertainties assessed in the current work include variances in the decay heat, total power, graphite specific heat, conductivities and emissivities, and bypass flows. The characterization of bypass flows in HTGRs is an important element in the accurate prediction of core and reflector temperatures, specifically during a loss of forced cooling (LOFC) transient (Johnson et al. 2009). As a first-order approximation, it is common to simulate the heat distribution with a network of one-dimensional (1D) pipe-flow models and two-dimensional (2D) heat-conduction heat structures. The dominant heat-transfer mechanism during normal operating is convective heat removal via the forced helium flow and radial heat conduction between the fuel and reflector blocks. Radiation heat transfer in the gaps between blocks and across large gaps—such as the control-rod holes, the upper plenum and the reactor vessel and core barrel—is only dominant during an LOFC transient. The approach taken in this work for the RELAP5-3D modeling of the MHTGR-350 (Strydom 2016) is discussed in Appendix B-1.

In HTGR designs, graphite acts as a neutron moderator and provides structural support and protection during oxidation events. The MHTGR-350 design contains approximately 450 tons (250 m<sup>3</sup>) of graphite reflector blocks, as well as 80 tons of graphite in fuel blocks. The large thermal inertia of moderator graphite in the fuel and reflector regions leads to slow changes in the distribution of heat during LOFC transients. When the core enters a sub-critical state (e.g. following a reactor trip), the only heat source remaining is the decay of the short- and long-lived fission products. The fission-product decay-heat term is nominally around 8% of the total thermal power at the beginning of the depressurization event (e.g. 28 MW for the MHTGR-350). From there, it decreases to less than 1% within a few hours (Massimo 1976). It is shown in Section 7.5 that uncertainties in the decay heat are responsible for a significant contribution to the uncertainties in the PLOFC maximum fuel temperature.

## 2.2.4 The V&V of HTGR Codes and Models

*“Experimental results are believed by everyone, except the person who ran the experiment.*

*Computational results are believed by no one, except the person who wrote the code.”*

Max Gunzburger.

All neutronics and thermal fluid codes require V&V. Verification involves the characterization, reduction, and, ideally, elimination of numerical approximation errors associated with a simulation, and typically includes discretization, iterative convergence, and round-off errors, in addition to computer-programming mistakes. Validation is the assessment of a model accuracy by comparison of the simulation results with experimental data (Roy & Oberkampf 2011).

In the context of HTGR code-to-code verification, best-estimate code-to-code verification HTGR benchmarks were organized by the NEA on the Pebble Bed Modular Reactor (PBMR)-400 (OECD/NEA 2013) and MHTGR-350 (OECD/NEA 2018) designs, preceded by an earlier set of IAEA benchmarks on the Adaptierter Schwimmbecken-Typ-Reaktor Austria (ASTRA), HTR-10, Gas Turbine Modular Helium Reactor (GT-MHR) and PBMR-400 designs (IAEA 2013). Some of the benchmarks were used during the development of dedicated HTGR simulation tools—e.g. PEBBED<sup>6</sup> (Gougar et al. 2002) at INL and Purdue Advanced Reactor Core Simulator (PARCS)-Advanced Gas REactor Evaluator (AGREE) (Seker 2007)—while most recently, experimental HTGR data have been used to validate HTGR neutronics and thermal fluid simulations in modern large-scale platforms such as MAMMOTH<sup>6</sup> (Ortensi et al. 2018).

For LWR-simulation code validation, developers have access to the raw and processed measurement data from hundreds of operational power plants over the last 60 years, as well as many dedicated separate-effects and integral test facilities—e.g. the PWR Main Steam Line Break Benchmark (OECD/NEA 1999) and Virtual Environment for Reactor Analysis Validation Plan (Godfrey 2014). The data sets typically include detail on the flux, power, temperature, and other critical parameters used in core design, safety analysis, and licensing. This situation is very different for HTGRs, where very few experimental or operational data sets exist that can be used for the separate-effects or integral validation of simulations. The Advanced Reactor Technologies HTR Methods Technical Program Plan (Gougar 2016) describes the development of a validation matrix for HTGRs based on the identification of equations that describe each domain along with the design of integral and separate-effects experiments available for validation. In addition, validation surveys have been performed by Korean Atomic Energy Research Institute (KAERI) (2004), the U.S. NRC (2009), and ANL (Taiwo et al. 2005) to identify the limited existing data sets that could be used for HTGR neutronics and thermal fluid code validation. Table 2-4 provides an example of

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<sup>6</sup> Not an acronym.

## CHAPTER 2: HTGR DEVELOPMENT AND SIMULATION

how these historical data sets can be reviewed to determine their suitability for HTGR U/SA validation. The table shows that some data sets are either not available in the public domain, are marginally applicable to modern designs, or are too limited to be used for U/SA validation. The VHTRC and HTR facilities produced data sets that enabled the production of formal benchmark definitions and include some estimates of uncertainties. They therefore represent the best options for the quantification of cross-section uncertainties on prismatic HTGR neutronics. Based on this lack of HTGR validation data, an argument is made in Section 3.1.2 that deterministic U/SA methods that require large measured data sets as input cannot currently be applied to the HTGR domain. This factor is an important reason why the statistical methodology is seen as the only viable HTGR U/SA option for the foreseeable future, especially if the absence of current experimental or operational HTGR programs is considered.

Table 2-4. Examples of experimental and operational HTGR data.<sup>7</sup>

| Description              | Data Status                                                                                                         | Applicability to HTGR Validation <sup>8</sup> | Uncertainty Data Available? <sup>9</sup> |
|--------------------------|---------------------------------------------------------------------------------------------------------------------|-----------------------------------------------|------------------------------------------|
| Dragon, UK               | Some public, most detail data are limited.                                                                          | Low                                           | No                                       |
| HTR, Japan               | Early data public, later data proprietary (IAEA, 2003).                                                             | High                                          | Yes                                      |
| VHTRC, Japan             | OECD/NEA International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhEP) (OECD/NEA, 2006b).      | High                                          | Yes                                      |
| Peach Bottom 1, USA      | Early physics tests public, operational global and ex-core data limited, in-core data proprietary.                  | Low                                           | No                                       |
| Fort St Vrain, USA       | Early physics tests public, operational global and ex-core data limited, in-core data proprietary.                  | Medium                                        | No                                       |
| HTR-PROTEUS, Switzerland | IRPhEP benchmark (IRPhEP) (Bess et al. 2014).                                                                       | High                                          | No                                       |
| NSTF & HTTF, USA         | Public-domain heat-transfer data of air- and water-cooled reactor-cavity cooling system (RCCS) and LOFC performance | High                                          | Yes                                      |

<sup>7</sup> This list is limited to data that could be applied for *prismatic* HTGR validation. For example, the SANA experiment was limited to pebble fuel only, but the PROTEUS facility could generate data for both pebble and block fuel.

<sup>8</sup> The suitability of the data set for validation of LEU-fueled HTGR best-estimate calculations (high, medium, low).

<sup>9</sup> Can the data set can be used for validation of uncertainty and sensitivity assessments? In addition to nominal data, estimates of measurement, material, and operational uncertainties are required (typically, one sigma).

### 3. UNCERTAINTY AND SENSITIVITY ASSESSMENT METHODOLOGY AND PROPOSED APPLICATION TO THE IAEA CRP ON HTGR UAM

*“With thermodynamics, one can calculate almost everything crudely; with kinetic theory, one can calculate fewer things, but more accurately; and with statistical mechanics, one can calculate almost nothing exactly.” Eugene Wigner.*

In this chapter, the BEPU approach is used as the departure point for a survey of some of the uncertainty and sensitivity methodologies developed over the last 15 years. Because the focus of the present research is the novel application of an existing U/SA methodology approach to the coupled transient analysis of prismatic HTGRs, the discussion in Section 3.1 specifically focusses on work that has been done thus far on the combined impact of neutronic and thermal fluid uncertainties. In Section 3.2, the U/SA methodology proposed for the research is motivated primarily based on a lack of sufficient V&V data for HTGRs, and the need for a robust solution for the complex, non-linear nature of coupled multiphysics transient simulations.

#### 3.1 The use of BEPU Analysis for HTGR Design and Licensing

The MHTGR-350 Preliminary Safety Information Document (PSID) (Stone & Webster Engineering Corporation 1986) lists several transients that vary in frequency of occurrence (e.g. a PLOFC is caused by a turbine trip, which can occur more frequently than a DLOFC, which is a break in the pressure boundary) and the consequences (e.g. there is no fission-product release outside the pressure boundary during a PLOFC). Transients such as the PLOFC and CRW events are defined as design-basis accidents, and the reactor designers are required to show the effects of these transients on typical safety FOMs, such as the local power peaking, fuel temperature, and control-rod worth.<sup>10</sup> The designers are also constrained by the limiting values that exist for the various materials and components that are used in the design (e.g. a limit on the reactor pressure vessel [RPV] peak temperature). The difference between the calculated magnitudes of the FOMs that are experienced during accident scenarios and the limiting values of the selected FOMs are “margins” of safety in the design, or the level of “conservatism”. The nuclear regulator would typically require that because there are always uncertainties in any code simulation, as well as the experimentally determined safety limits, the reactor designers provide proof of acceptable safety margins.

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<sup>10</sup> Although this work is focused on reactor-analysis parameters like fuel temperature, eigenvalue, and power peaking, the ultimate FOMs for safety and licensing analyses are the worker and public dose that results from each of these accidents.

The safety margin is defined as the difference between the best-estimate value and the safety limit. This design and licensing philosophy is commonly referred to as BEPU analysis, with best estimate (BE) the nominal simulation code results, and the uncertainty (U) that is added (P, for plus) to the BE result. The relationship between these varied concepts are shown in Figure 3-1. The focus in this work is on the first arrow from the bottom—i.e. the assessment of uncertainties in best-estimate HTGR models.

A second important reason for the assessment of nuclear-data uncertainties is that the output of these studies is used by the community to recommend areas where refined measurement or models would likely lead to a reduction in data uncertainties, which benefits the new generation of simulation tools currently under development.

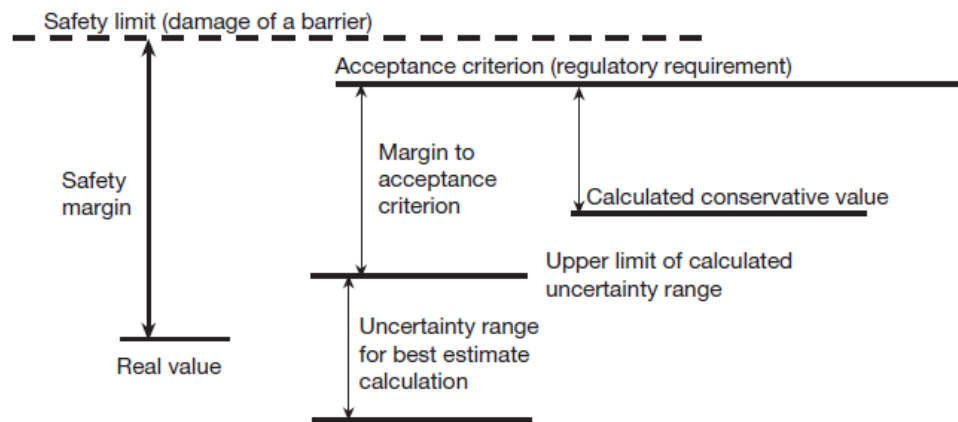


Figure 3-1. Uncertainties and safety margins (IAEA 2008).

An excellent historical review of the development of BEPU safety analysis is provided by Wilson (2013); he notes the differences between BEPU and the conservative approach commonly followed up to the late 1970s, when input parameters and models were purposely adjusted to produce conservative predictions. The BEPU approach is also the core element of large-scale international projects such as Best Estimate Methods, Uncertainty and Sensitivity Evaluation (BEMUSE, OECD/NEA 2011) and the OECD/NEA UAM (OECD/NEA 2013–2017) and is described in detail in the IAEA Safety Series Report on uncertainty methods (IAEA 2008) and the U.S. NRC Regulator Guide 1.203 (U.S. NRC 2005). A recent paper of the role of V&V in BEPU development (Zhang 2019) provides a comprehensive overview of the latest BEPU landscape and advocates for a pragmatic and graded approach to make full use of the advantages the BEPU approach can provide to the industry.

Ivanov et al. (2018) emphasize that although U/SA research and the development of propagated BEPU methodologies have been very active in the last few years, the use of BEPU for actual licensing decisions has been limited so far.

In addition, the authors stress the important caveat that “. . . BEPU heavily depends on the availability of representative and accurate experimental data, e.g. on suitable validation sets of experiments”. This critical aspect of BEPU is one the major stumbling blocks for the assessment of HTGRs because high-quality V&V data that cover all phenomena relevant to neutronics and thermal fluids are very limited and certainly insufficient. In the HTGR domain, none of the historical facilities were licensed using the BEPU approach, but a new applicant would nevertheless need to follow the latest NRC requirements on BEPU analysis.

### 3.1.1 Sources of Uncertainties

In general, sources of uncertainties can be classified into two groups (Palmiotti and Salvatores 2013, Hoffman and Hammonds 1994):

- Aleatory (stochastic/irreducible) uncertainties are related to the inherent variations in the system under consideration and are irreducible. These typically include uncertainties in measurement, manufacturing processes, reactor operational conditions, etc.
- Epistemic (subjective/reducible) represents a lack of knowledge in any component of the modeling process and can be reduced or even eliminated, based on additional information. A lack of experimental validation data and numerical approximation can be classified as epistemic uncertainties, since both can be improved by obtaining more data or selecting better approximations.

A typical nuclear reactor analysis contains aleatory and epistemic uncertainty sources and a mixture of both. It should be noted that the classification above simplifies the complex relationship that exists between these sources of uncertainty. For example, Jakeman (2010) notes that “. . . the sources of aleatory uncertainty include both uncertainty in model coefficients (parametric uncertainty) and uncertainty in the sequence of possible events (stochastic uncertainty)”. In addition, an epistemic uncertainty can provide conservative bounds on an underlying aleatory uncertainty, which can converge to the true aleatory uncertainty if sufficient additional information can be found. Whereas aleatory uncertainties are typically quantified by probability density functions (PDFs), if enough information is available, epistemic uncertainty can be represented as either an interval with no associated PDF, or a PDF which represents “...the degree of belief of the analyst” (Roy and Oberkampf 2011).

Two examples of this type of epistemic uncertainty in the current work is the choice of few-group energy structures for HTGR core analysis or the choice of a specific-heat-transfer correlation over another available correlation.

By selecting more groups (e.g. 26 vs. 2), the spectral effects of material variations and self-shielding can be captured more accurately, but unless a very fine group structure (200–1000) is chosen, the uncertainties are only reduced, not eliminated.

Likewise, more than one correlation might fit the same experimental data set, but with different uncertainty margins that are propagated through the analysis chain. In general, estimates of the impacts on epistemic uncertainties are not included in this work although some aspects are discussed in Chapters 4–8.

“User” effects play a significant, but difficult to assess role in uncertainty quantification. Ivanov et al. (2018) note the large impact that “user choice”—e.g. choice of simulation code, model nodalisation, number of samples or material-property correlations—had on benchmark results. At the 2015 Research Coordination Meeting of the IAEA CRP on HTGR UAM, the  $k_{\infty}$  variances between the participants “blind” Phase I results (i.e. before comparisons were shown) were larger than 1,000 pcm, compared to ~600 pcm for the cross-section uncertainties. These were mostly attributed to incorrect interpretation of the problem specifications, model input errors and insufficient spatial mesh refinement. Computational uncertainties can usually be quantified by comparison with an independent code, e.g. a three-dimensional (3D) Monte Carlo code vs. a 2D deterministic nodal code.

### 3.1.2 Review of Current U/SA Methodologies

In this section, a summary of recent developments in the field of uncertainty and sensitivity assessment methodologies is provided. This summary is not intended to be exhaustive, but rather to motivate the selection of the statistical approach for the HTGR U/SA reported in the current work. Because the development and application of U/SA methods has been a very active research area for the last 15 years, several comprehensive summary surveys can be found in the literature.

Very few of these publications, however, includes applications to HTGRs; most are applied to water-cooled systems. The detailed review paper by Salvatores et al. (2014) on a NEA/OECD fast-spectrum collaborative study of the combined use of integral experiments and nuclear-covariance data is a good example of the effort that is needed for HTGR systems as well. The summary publication by Rochman et al. (2017) on the depletion studies performed for an LWR assembly and core is likewise representative of the current state of the art in thermal-spectrum U/SA.

Interest in the use of nuclear-covariance data for reactor applications has been increasing since the 1970s; some of this earlier work include an ORNL report on U/SA theory and applications (Weisbin 1978) and an ANL report on the use of covariances (Smith 1981). One of the few HTGR publications from this era is from an IAEA specialist meeting on uncertainties in HTGR-physics calculations (IAEA 1991).

A paper by A. Baxter (2010) contained in this report lists the results of a survey performed on historical Fort St Vrain and Peach Bottom data, from which the GA team concluded that the experimental data base is adequate to ensure that the MHTGR temperature coefficient of reactivity can be calculated with an uncertainty of 20%, the control-rod worth within 10%, and local power distributions within 13%.

These estimates seem large when the fidelity of modern predictive tools is considered, but the GA team made the point that the experimental data that provide the validation basis for HTGR simulation tools *do not allow* lower uncertainty estimates. Although the HTGR validation landscape did improve somewhat since then (with data from the HTTR, HTR-10, etc.), the lack of applicable LEU HTGR experimental data for both neutronics and thermal fluids is indeed still a significant issue, and a limitation on the use of modern HTGR tools because their accuracy cannot be fully validated.

As indicated previously, the various input uncertainties (described in Section 2.3.2) lead to uncertainties in the eventual output parameters of the reactor model. The propagation of these input uncertainties through the various phases of HTGR reactor simulation and the characterization of the impact on important FOMs are the foci of this research. The objective of *uncertainty* analysis is to assess the effects of input-parameter uncertainties on the uncertainties in computed results, and specifically for a predefined set of FOMs related to design optimization or safety studies. The objective of *sensitivity* analysis is to quantify the effects of input-parameter variations on computed results.

In general, the propagation of uncertainties can be treated using deterministic or statistical approaches. The deterministic and statistical U/SA methods define inverse roles for the quantification of sensitivities and uncertainties; in the deterministic method, sensitivities are first quantified to inform the selection of parameters for the uncertainty quantification while the statistical method first performs an uncertainty study on all parameters of interest and then quantifies the sensitivities for each of the uncertain input parameters on the FOMs. Both methods require the formulation of ranges and PDFs for all input uncertainties.

These terms were, however, not always consistently applied in the community, as was pointed out by Ionescu-Bujor and Cacuci in their two-volume comparative review of deterministic and statistical <sup>11</sup> sensitivity and uncertainty analysis for large-scale systems (Ionescu-Bujor and Cacuci 2004). A generic process flow of the statistical uncertainty propagation methodology is shown in Figure 3-2. The main steps, advantages and disadvantages of the two methods can be summarized as follows (from Ionescu-Bujor and Cacuci 2004):

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<sup>11</sup> The authors use *statistical* to describe the type of U/SA method, and *stochastic* to describe a type of randomly occurring uncertainty. This convention will be followed here as well.

- Statistical U/SA
  - Steps
    - Step 1: Define distributions to characterize uncertainties in a *limited* number of input parameters.
    - Step 2: Generate a sufficient number of samples ( $N$ ) from the input-parameter distributions and generate  $N$  input decks to use in the simulation model.
    - Step 3: Perform  $N$  simulation calculations to obtain acceptable statistics.
    - Step 4: Perform an uncertainty analysis of the desired responses (FOMs) by determining the mean and variance of the sample, for example.
    - Step 5: Perform sensitivity analysis of the responses by using scatter plots, regression and correlation analysis, etc., to assess the impact of the variations in input parameters on the output.
  - Advantages
    - Because it is applied to the input parameters of models, there is no need to modify the simulation code source itself (i.e. it is non-intrusive). An external “wrapper” approach can be followed, consisting of an external code that interfaces with the simulation code via perturbation of the input-file parameters. It is therefore faster and cheaper to implement.
  - Disadvantage
    - A sufficient number of (possibly expensive) model realizations must be performed to obtain acceptable statistics.
- Deterministic U/SA
  - Steps
    - Step 1. Perform a sensitivity analysis to identify the dependence of a response/FOM on the simultaneous variation in *all* uncertain input parameters.
    - Step 2. Combine the individual sensitivities in an uncertainty analysis to predict the overall uncertainty.
  - Advantages
    - No knowledge is required on the uncertainties of the input parameters.

- Typically, only one solution is required per response to determine all sensitivity coefficients and uncertainties (e.g., the Contribution-Linked eigenvalue-sensitivity/Uncertainty estimation via Track length importance CHaracterization (CLUTCH) method in SCALE).
- Disadvantages
  - The method requires applicable experimental data.
  - The method is intrusive, i.e. modifications are required to the simulation code source to include generalized adjoint perturbation capabilities. These adjoint calculations need to be repeated for each response/FOM.
  - The adjoint produces a linear approximation to the output parameter probability distribution function. For thermal-hydraulic problems, the true distribution may be significantly non-linear (Briggs 2008), but recent research in this area produced promising results (Cacuci 2014, Cacuci et al 2016).

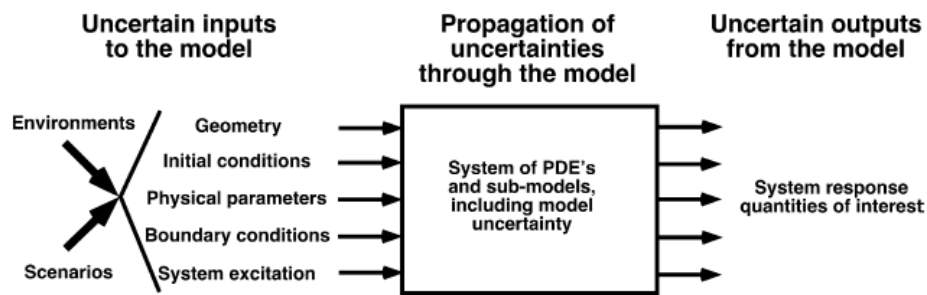


Figure 3-2. Non-deterministic (statistical) propagation of input uncertainties to obtain output uncertainties (Roy and Oberkampf 2011)

In the U/SA community, most approaches for quantifying uncertainties in best-estimate model predictions are based on statistical methods. A non-parametric approach is usually followed in which all uncertain parameters are sampled simultaneously, and the number of samples is decoupled from the number of uncertain input parameters. In this manner, a few hundred samples can be generated out of the simple random or stratified Latin hypercube sampling of thousands of nuclides and reaction types.

A frequently listed disadvantage of the statistical methodology is the computational resources required to perform a sufficiently large number of lattice- and core-model perturbations. A typical core calculation can take several hours (or even days) to complete on a single processor, depending on the number of energy groups and the spatial resolution of the model, and between 100–1,000 core calculations are usually required to ensure good statistics for multiple models and at multiple simulation stages.

This computational burden can, however, be largely mitigated using *parallel* processing on small to medium clusters (i.e. ranging between 50–500 processors), where many perturbed simulations can be performed simultaneously. Because increasingly affordable access to either in-house or cloud-based high-performance clusters is becoming more common at research organisations, universities, and commercial core designers, this drawback is not seen as a major hurdle for the implementation of the proposed statistical U/SA option.

Examples of recent applications of the statistical U/SA method include the Software for Uncertainty and Sensitivity Analysis (SUSA) (Jaeger et al. 2017) and cross-section uncertainty and sensitivity analysis (XSUSA) (Williams 2013) packages developed at Gesellschaft für Anlagen und Reaktorsicherheit (GRS), NUSS-RF at PSI (Zhu et al. 2015), NUDUNA by AREVA (Buss et al. 2011). In the U.S. the DAKOTA (Adams et al. 2016) code was developed at Sandia National Laboratories (SNL) and the RAVEN (Rabiti et al. 2013) at Idaho National Laboratory (INL). The GRS team also published a recent paper (Aures et al. 2019) utilizing the SCALE/Sampler sequence applied to BWRs and an LWR mini-core problem.

In the HTGR domain, a study on decay-heat uncertainties has been performed with RAVEN (Alfonsi 2018), and the full coupling of RAVEN, SCALE, and the transient core code P/R (Rabiti et al. 2016) was completed as a joint project between INL and North Carolina State University (NCSU) for the IAEA CRP on HTGR UAM (Rouxelin 2019). For prismatic HTGRs, the Korean (Han et al. 2015, Han et al. 2019) Russian (Boyarinov et al. 2017) and South African (Sihlangu et al. 2018; Sihlangu, et al. 2019) participants in the IAEA CRP applied both deterministic and statistical methods in their assessment of Phase I and II results, most of which will be discussed in Chapters 3 and 4 in relation to the work performed here. A detailed listing of the author’s publications related to the HTGR UAM is included in Appendix C as Table C-1.

In addition to the prismatic HTGR research listed above, a few recent studies by Kim et al. (2018), Wang et al. (2014), Hao et al. (2018), and Liu et al. (2018) applied the statistical method on the neutronics of pebble-bed reactors.

Deterministic methods have not been widely used so far outside nuclear-data applications because they depend on extensive high-quality experimental data from separate effect and integral experiments, and the implementing the adjoint formulations in existing core-physics and thermal fluid codes. Examples of recent applications of the deterministic U/SA method include the predictive modeling of coupled multiphysics systems method (Cacuci 2014), the use of Bayesian analysis to establish inverse U/SA problems based on experimental data, with systematic and rigorously derived surrogate models based on polynomial chaos expansion (Wu and Kozlowski 2017), and the extended GPT method that applied the GPT capabilities of Monte Carlo codes to CE sensitivity functions (Aufiero et al. 2016).

According to the author’s knowledge, the only adjoint-based study focused on the HTGR domain was published by Drzewiecki (2013). In this work, he implemented the adjoint method into the NRC AGREE code and tested surrogate models using DAKOTA. His application was demonstrated on experimental facilities related to the HTTR, as well as data from the HTTR itself. Availability of these experimental data sets was a key factor in his successful implantation and testing of this approach into AGREE.

Two promising developments for multiphysics sensitivity analysis that could combine both statistical and deterministic methods without the need of code modification are the efficient subspace method (Abdel-Khalik et al. 2008), and the quasi-Monte Carlo randomized sampling suggested by Anitescu et al. (2007).

Based on the arguments listed below, the statistical U/SA method is selected to investigate the uncertainties and sensitivities related to multi-phase and multiphysics transient analysis of the prismatic MHTGR-350 design:

- As discussed in Section 2.2.4, HTGRs typically lack an extensive experimental and operational data base that is applicable for modern ~8–20% enriched HTGR designs. This fact, *by itself*, disqualifies the deterministic U/SA method as an option for coupled transient analyses of HTGRs because the deterministic method requires good-quality experimental uncertainty data as part of the U/SA process.
- Adjoint solutions for coupled non-linear parameters—such as the effect of uncertainties in graphite density, temperature, and fluence on graphite thermal conductivity during an LOFC transient or the relationship between graphite swelling, bypass flows, and fuel temperatures—do not yet exist, and might require extensive resources to develop, if that is at all possible.
- Even if the adjoint formulations can be developed for neutronics, the implementation of thermal fluid adjoint solvers in a well-established and tested systems code such as RELAP5-3D is a significant undertaking, compared to the “black-box wrapper” statistical U/SA method. Very few users will obtain source-code access to RELAP5-3D.
- Similar statistical U/SA schemes using different lattice and core codes have already been applied to LWRs and BWRs (Hernández-Solís 2012, Bielen 2015, Melia 2017, Zeng, et al. 2018). These schemes were successfully validated using much-larger experimental or operational LWR datasets than those available to HTGRs.

## 3.2 Application of the Statistical U/SA Methodology to the IAEA CRP on HTGR UAM

In Section 3.2.1, an overview is provided of the IAEA CRP on HTGR UAM, which was developed as a major contribution of this research, to demonstrate the viability of the proposed statistical U/SA methodology. It should be stressed that the chosen methodology described in Section 3.2.2 is agnostic to specific simulation codes; for the work reported in this dissertation, the assessment of the MHTGR-350 modeling uncertainties and sensitivities, INL-developed codes PHISICS, RELAP5-3D and RAVEN were chosen to provide a practical example of the methodology implementation.

### 3.2.1 Overview of the IAEA CRP on HTR UAM

Following on the BEMUSE set of benchmarks, the OECD/NEA launched the current LWR UAM series of benchmarks (OECD/NEA 2013–2017), which later included exercises for Vodo-Vodyanoi Energetichesky Reactor (VVER), BWR and sodium-cooled fast reactor (SFR) designs. Because HTGR systems were not included in the OECD/NEA effort, the IAEA launched a CRP on HTGR UAM to investigate the propagation of uncertainties and determine sensitivities for prismatic and pebble-bed HTGRs (Reitsma et al. 2012). The overall objective of the IAEA CRP on HTGR UAM is to assess cross-section, boundary-condition, material-property, and manufacturing-input data uncertainties and, specifically, their impacts on the lattice, core and system simulation results of pebble bed and prismatic HTGR systems.

The prismatic specifications were developed by the author as principle investigator, with support provided by Friederike Bostelmann of ORNL and Pascal Rouxelin of NCSU in the period 2014–2018. It is seen as one of the major contributions of the Ph.D. research reported in this dissertation.

To leverage previous work performed by some of the participants on the OECD/NEA MHTR-350 benchmark, it was decided to use those works' the basic information on geometry, material compositions, and operational conditions, as described in Appendix A. However, it is important to note that although the same reactor-design information is used for both the OECD/NEA and IAEA CRP benchmarks, the definition of the core states differs significantly. For the OECD/NEA benchmark, the end of equilibrium cycle nuclide data was obtained from GA. No fresh-core case was defined, and the mixed core consisted of 220 fuel blocks that were shuffled and reloaded after one and two burn cycles, respectively. Each of the 220 fuel blocks (22 fuel blocks in 10 axial layers) had unique nuclide composition and, therefore, cross-section libraries, based on their specific exposure histories.

In contrast to this, the IAEA CRP on HTGR UAM simplified this approach by specifying a fresh core that consisted only of fresh fuel everywhere for Exercise II-2a (i.e. a single cross-section and isotopic data set), as well as a mixed core that contained fresh and depleted fuel blocks (Exercise II-2b) in 10 identical

axial core layers. Although the mixed-core packing pattern is the same for both benchmarks (Figure A-4), the depletion state of the burned blocks is not the same. The final important difference is that OECD/NEA participants all used the same provided cross-section set while IAEA CRP participants are requested to generate their own Phase II cross-sections from the respective lattices they used in Phase I. Direct comparisons of eigenvalues, power densities, and temperatures between the two benchmarks are therefore not possible.

### ***Phase I: Local (Cell and Lattice) Neutronics and Thermal-Fluid Calculations***

Exercises I-1 and I-2 are focused on the derivation of the MG and few-group microscopic cross-section libraries. The objective is to address the uncertainties due to the basic nuclear data, as well as the impact of processing the nuclear and covariance data, selection of MG structure, and double-heterogeneity or self-shielding treatment. The intention is to propagate the uncertainties in evaluated nuclear-data libraries (i.e. microscopic point-wise cross-sections) into MG microscopic cross-sections and to propagate the uncertainties from the MG microscopic cross-sections into the few-group cross-sections for use in Phase II. Exercise I-1a consists of a homogeneous fuel region of homogenized TRISO fuel particles and matrix graphite whereas Exercise I-1b requires the explicit modeling of the TRISO fuel particles to investigate their self-shielding effect on the MG microscopic cross-sections.

Exercise I-2a requires a lattice calculation to be performed on a single fuel block at hot full-power (HFP) conditions while Exercise I-2b specifies the same problem at 100 MWd/kg-U burnup. Exercise I-2c adds the spectral effects of the neighbouring domain by performing a lattice calculation on a supercell, which consists of a fresh fuel block surrounded by a mixture of depleted and fresh fuel on one side and graphite reflector blocks on the other side. This calculation is also performed at HFP conditions.

Exercises I-3 and I-4 are focused on the localized stand-alone fuel thermal response. The aim of the stand-alone thermal-unit cell calculations is to isolate the effects of material and boundary input uncertainties on very simplified problems before the same input variations are applied to complex core problems (e.g. Phases II and III). Exercise I-3 requires a steady-state solution for a single fuel compact and coolant-channel unit cell with a fixed bulk-coolant temperature. Two subcases, similar to Exercise I-1, are again defined here, taking into account the explicit modeling of heat transfer from the TRISO fuel particles to the matrix graphite. Exercise I-4 uses the same unit cell definition as described for Exercise I-3, but a time-dependent power excursion is prescribed, as opposed to constant steady-state power.

### ***Phase II: Core Stand-alone Calculations***

The global (or core) exercises defined for Phase II use cross-section libraries generated in Phase I as the propagated input data. All Phase II calculations are performed at HFP (1,200 K) conditions, and are defined as follows:

- **Exercise II-1: Neutronics—block and core depletion.** As the first variant of the depletion cases, the single block defined in Exercise I-2a is depleted up to 80 GWd/MTU as Exercise II-1a. For Exercise II-1b, a full-core depletion to the same burnup is requested.
- **Exercise II-2: Neutronics—stand-alone core steady-state.** Two full-core steady-state neutronics calculations at HFP conditions are performed using the given fresh (Exercise II-2a) and mixed (Exercise II-2b) core number densities, respectively. The fresh-core model is identical to the starting point for Exercise II-1b if participants elected to perform the depletion cases. The cross-section libraries developed in Exercise I-2 should be utilized for this core calculation.
- **Exercise II-3: Neutronics—stand-alone core kinetics without feedback.** This exercise involves a full-core calculation with reactivity being added and then returned to normal at HFP conditions, but without any temperature feedback. The reactivity-induced transient is defined as control-rod movement at normal speed to ensure that the delayed neutrons play a role (i.e. no prompt-critical effects). The uncertainties in the kinetic parameters are added in this case, and only the mixed (fresh and depleted) core loading is considered.
- **Exercise II-4: Thermal fluids—stand-alone core steady-state.** The conditions at normal HFP operation are considered with the reactor-core power distribution specified. No neutronics feedback exists.

### **Phase III: Coupled Steady-State**

Exercise III-1 requires a coupled calculation focused on the steady-state HFP neutronics and thermal-hydraulics core performance. Many of the uncertainties determined in the previous stand-alone cases (Exercises II-2 and II-4) are propagated to this model. Only the mixed-core loading is considered.

### **Phase IV: Coupled Core Transients**

Exercise IV-1 is defined as a PLOFC transient. The forced-helium loss flow rate is terminated over 30 seconds. Because this is a subcritical event initiated by a turbine trip, neutronics feedback is optional. Exercise IV-2 is a coupled mixed-core transient at HFP conditions with full thermal (Exercise III-1) and kinetics feedback (Exercise II-3). It is defined as a reactivity-induced power excursion due to a control-rod withdrawal. The feedback effect from the rest of the power conversion unit is kept constant, (i.e. the focus is on the core response only). Only the mixed core version is investigated.

A visual representation of the HTGR UAM phases and exercises is presented in Figure 3-3. The figure also includes a mapping to the relevant sections in this dissertation where the exercises are discussed, while the arrows show the propagation of uncertainties and links between these exercises.

The scope of work included in this dissertation is limited to Ex. I-2, II-2, II-4, III-1 and IV-1. It was decided to focus the discussion in this work on the propagation of neutronics uncertainties from the Phase I lattice to the Phase II core models. The Phase I cell exercise results (Ex. I-1a-d, Ex. I-3 and Ex. I-4) are therefore not included here because the uncertainties from these exercises are not propagated further through the core phases in the current methodology. (A discussion of the results obtained for the Phase I cell exercises can be found in an INL report by Strydom, Bostelmann and Yoon [2015]).

Rouxelin (2019) reported extensively on the depletion results obtained for Ex. II-1 in his Ph.D. dissertation, and the core stand-alone kinetics was not selected because Sampler does not yet include the capability to perturb kinetics parameters in version 6.2.

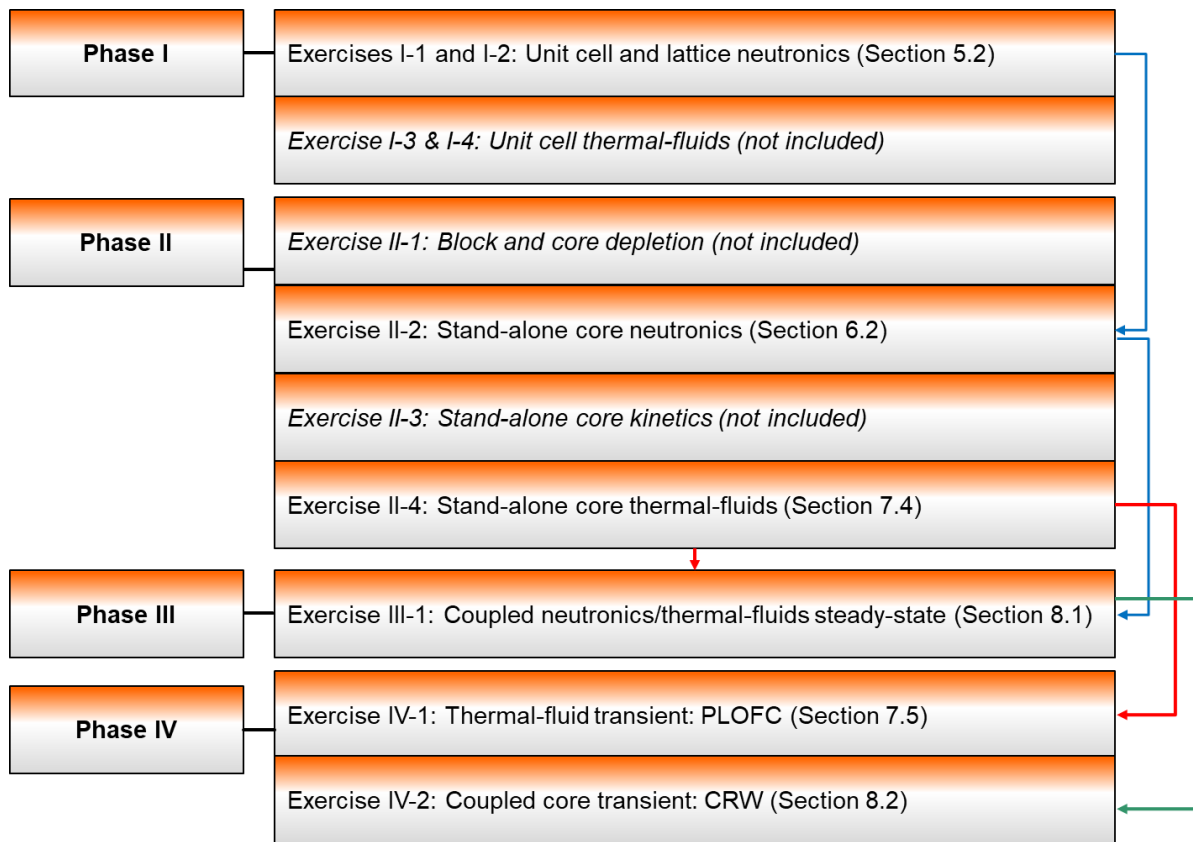


Figure 3-3. IAEA CRP on HTR UAM phases and exercises and mapping to dissertation section.

The primary contribution and focus of the current research is the propagation of uncertainties in both neutronics and thermal fluids to the coupled steady-state Ex. III-1 and the two Phase IV transients. Both of these transients were selected based on their typical inclusion in HTGR safety cases (Stone & Webster Engineering Corporation, 1986): the PLOFC is a high-frequency design basis transient initiated by the loss of off-site power, and the slow withdrawal of the control rod bank is likewise the limiting event for design basis reactivity insertion events.

The specifications were developed between 2014-2019 as part of the current research and released as three INL documents for review and acceptance by the CRP participants. The Phase I specifications and exercises are described in INL/EXT-15-34868 (Strydom and Bostelmann 2017), the Phase II-1 depletion specifications and INL nominal results in INL/LTD-17-41017 (Rouxelin and Strydom 2017), and the remaining Phase II exercises in INL/EXT-18-44815 (Strydom 2018). Although it was planned to release the Phase III and IV specifications in 2019 as well, IAEA support for the CRP was terminated in June 2019, and the specifications are currently only detailed as part of this dissertation in Sections 7.5, 8.1 and 8.2. It is expected that the forthcoming IAEA TECDOC will contain all the information for Phases I-IV in a single volume.

The focus in the HTGR UAM to date has been on the propagation of cross-section and material-data uncertainties; no coupling with thermal fluid codes or transient calculations have so far been reported by either the pebble or prismatic exercise participants. As indicated in Chapter 1, the research reported in this dissertation was sponsored by the U.S. DOE and represents the author's contribution to the IAEA CRP on HTGR UAM (as detailed in Table C-1).

### **3.2.2 Applied Stochastic Uncertainty Propagation Methodology**

The statistical U/SA methodology selected for this research is implemented using two established codes developed over decades at ORNL (SCALE) and INL (RELAP5-3D), and two INL codes developed over the last seven years (PHISICS and RAVEN). This work builds on, and is complimentary to, the coupling of RAVEN with the SCALE and P/R codes completed by Rouxelin (2019) as a joint research project between INL and NCSU. Rouxelin illustrated the use of the statistical methodology and the coupled toolset on the neutronics and depletion U/SA of prismatic HTGRs. The research reported in this dissertation extends the application of RAVEN, SCALE, and PHISICS to include the RELAP5-3D thermal fluids component and completes the coupled transient-analysis chain.

Uncertainties and sensitivities contribute in different ways to the state of knowledge. For safety and licensing purposes, uncertainties are more important because they provide information on safety margins. Sensitivities are important to the R&D community and basic data providers because they focus attention on where limited funds should be spent to improve the state of knowledge. The focus of Chapters 4–8 is on the contribution of this work to HTGR core designers and industry; therefore, the uncertainty assessment receives more attention than the sensitivity assessment in this dissertation.

The codes are used in the capacities listed below and summarized in Table 3-1. Descriptions of the codes' main features are provided in Appendix B.

- *Cross-section generation and lattice:* The perturbed cross-sections and lattice 8- and 26-group libraries are generated with the SCALE 6.2 Cross (X) Section Processing (XSProc)/NEWT/Sampler sequence (Bostelmann et al. 2018), utilizing the SCALE ENDF/B-VIII.1 252-group and 56-group covariance libraries.
- *Core:* The PHISICS code (Rabiti 2011) is used in stand-alone model for the neutronics-only cases of Phase II, RELAP5-3D (Balestra 2017) is used for stand-alone core thermal fluids, and the coupled version of the two codes P/R (Rabiti et al. 2016) is used for the Phase II and Phase IV steady-state and coupled transients.
- *U/SA:* Sampler (Williams et al. 2013) is used to create the perturbed cross-section libraries, and RAVEN (Alfonsi et al. 2017) to create the Phase II RELAP5-3D perturbed-input and overall U/SA analysis for all four phases.
- *Additional:*
  - Reference Phase I nominal calculations are performed using the KENO-VI and Serpent2 (Lepannen and deHart 2009) Monte Carlo codes.
  - The deterministic SCALE module TSUNAMI is used for CE sensitivity U/SA (Perfetti 2014) for the VHTRC (Chapter 4) and some of the Phase I exercises (Chapter 5).
- Table 3-1. Codes utilized in Chapters 5–8 for the MHTGR-350 U/SA.

| Code              | Role                                                                         | HTGR UAM application        |
|-------------------|------------------------------------------------------------------------------|-----------------------------|
| NEWT              | Deterministic nominal and perturbed transport solutions for cell and lattice | Ex. I-1, I-2                |
| Sampler           | Perturbed cross-sections                                                     | Ex. I-1, I-2                |
| KENO-VI           | Monte Carlo nominal and perturbed transport solutions for cell and lattice   | Ex. I-1, I-2                |
| Serpent2          | Reference nominal cell/lattice                                               | Ex. I-1, I-2                |
| TSUNAMI           | Reference nominal cell/lattice                                               | Ex. I-1, I-2                |
| PHISICS           | Core neutronics stand-alone                                                  | Ex. II-2                    |
| RELAP5-3D         | Core thermal fluids stand-alone                                              | Ex. II-4, IV-1              |
| PHISICS/RELAP5-3D | Coupled core neutronics/thermal fluids                                       | Ex. III-1, IV-2             |
| RAVEN             | Perturbed thermal fluids (RELAP5-3D), statistical metrics for U/SA           | Phases I-IV (all exercises) |

One of the primary features of the proposed methodology is that the codes used in this work can be exchanged for other tools capable of capturing the relevant physics of HTGRs. For example, Serpent2 can be used instead of the deterministic XSPROC/NEWT sequence for cross-section generation, and the core solvers P/R can be replaced with unstructured finite-element solvers like MAMMOTH (Ortensi et al. 2018) and Pronghorn (Zou 2017).

Likewise, a U/SA driver like DAKOTA (Adams 2016) can be used in the place of RAVEN. The use of established software tools with extensive pedigrees contributes significantly to the overall credibility of the U/SA results.

The general calculation scheme from the lattice Phase I to the transient Phase IV is presented schematically in Figure 3-4. The 2D deterministic transport code NEWT was used to construct various lattice models for the single fresh/depleted fuel blocks and a few supercell geometries for Phase I (see Chapter 3 for detail). The 252-group AMPX libraries were collapsed to 8 and 26 groups for use in the P/R Phase II core models, as described in Section 6.2.1.

A total of 1,000 perturbed lattice libraries were produced during the NEWT/Sampler sequence for each of the fresh, depleted, and supercell models described in Section 5.1, which in turn were used to calculate a set of 1,000 steady-state and transient-restart cases for each of the cores.

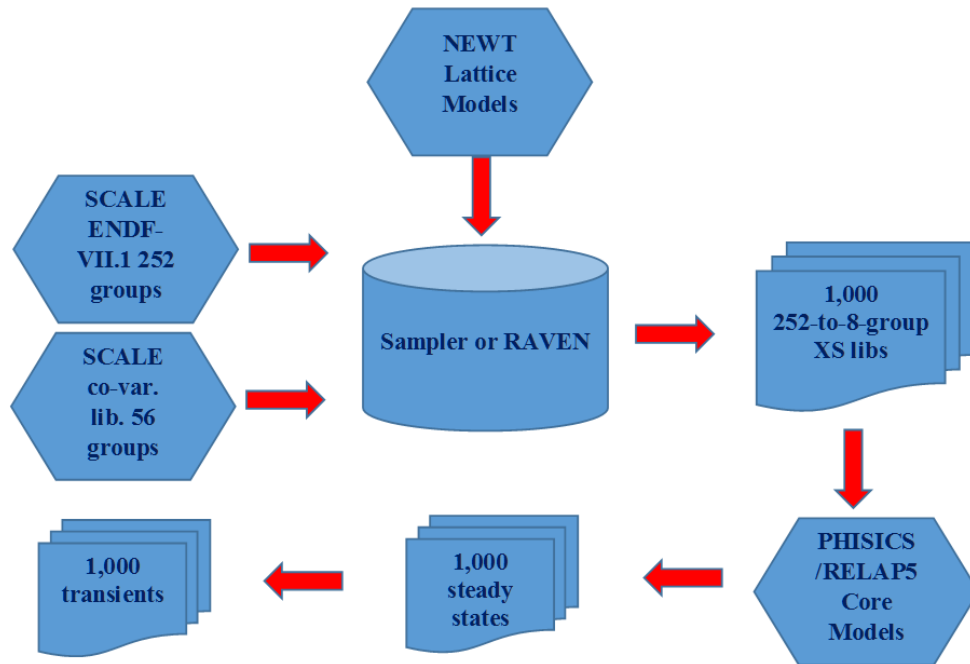


Figure 3-4. MHTGR-350 U/SA calculation flow scheme.

The XSProc microscopic libraries obtained from NEWT/Sampler are converted from the latest AMPX format (SCALE 6.2) to the older AMPX format (SCALE 6.1.3) because the cross-section interface developed for PHISICS can only use the older format AMPX libraries. The NEWT scalar flux is used to calculate disadvantage factors relative to each material and each group, after which the disadvantage factors are implemented in the PHISICS cross-section libraries. A flow chart of the calculation sequence developed by Rouxelin (2019) is given in Figure 3-5.

Disadvantage factors are used to correct for the spatial self-shielding effects that are present in the homogenized 8-group fuel-block libraries that are created from the heterogeneous detailed 252-group block solutions, and also to account for the spectral effects induced by the supercell, reflector, and control-rod blocks surrounding the fuel blocks (Rouxelin, 2019). The disadvantage factors are calculated with Equation 3-1. In the final step, the corrected 8-group microscopic library can be used in the PHISICS/RELAP5-3D core simulation. This process is repeated for each of the 1,000 perturbed libraries created by Sampler.

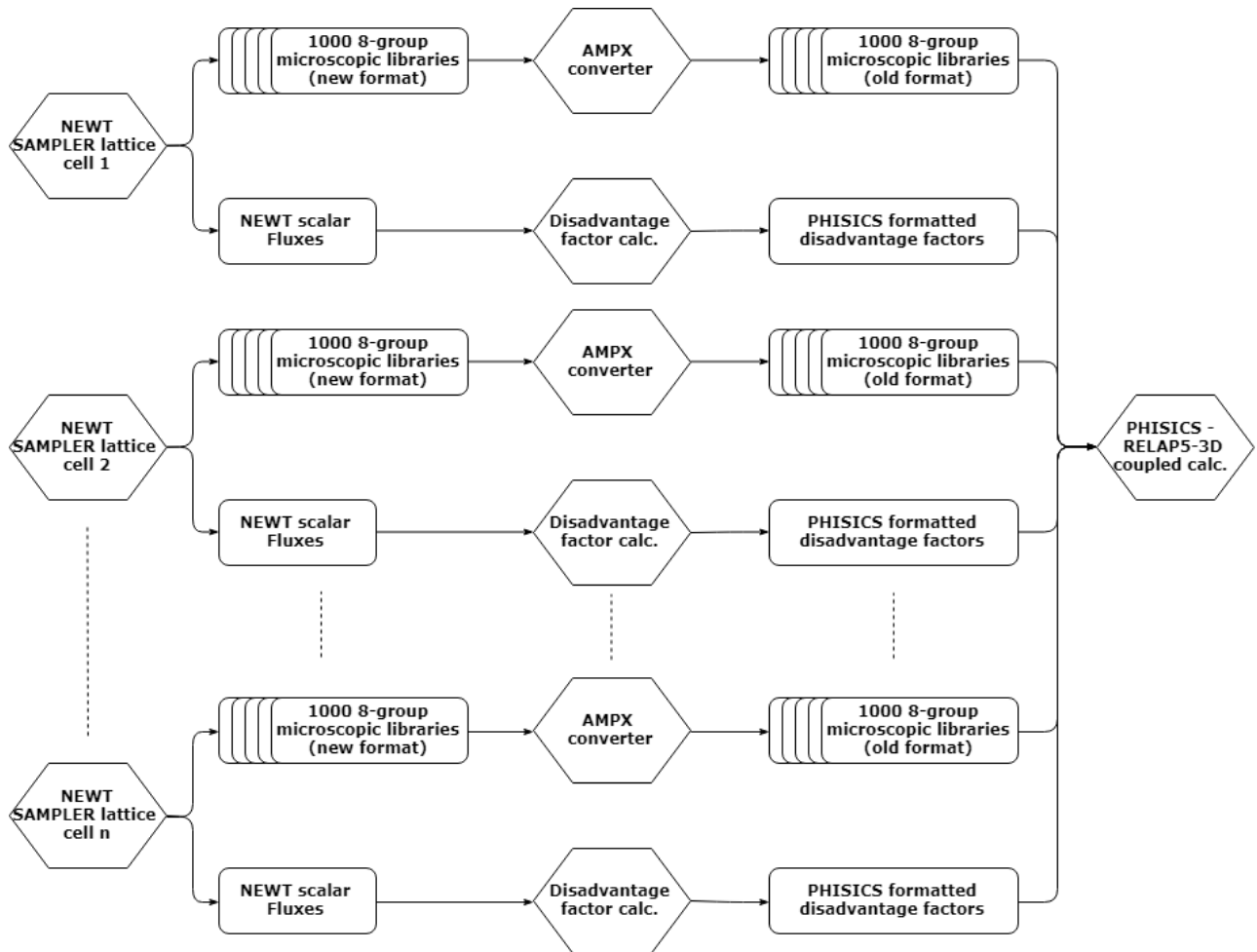


Figure 3-5. NEWT 252-to-8 group cross-section library generation flow scheme (Rouxelin, 2019).

$$d_g^m = \frac{\Phi_g^m}{\frac{\sum_{i=0}^M \Phi_g^i V^i}{V}} \quad (3-1)$$

where

$m$  = material mixture number,

$g$  = group number,

$\Phi_g^m$  = scalar flux in mixture  $m$  and energy group  $g$ ,

$V^i$  = volume of mixture  $i$ , and

$V$  = total lattice homogenized volume of a single fuel block (excluding the homogenized region of the supercell).

Sampler is a SCALE 6.2 “supersequence” that performs general uncertainty analysis by statistically sampling uncertain parameters that can be applied to any type of SCALE calculation propagating uncertainties throughout a computational sequence. It currently treats uncertainties from nuclear data (e.g. cross-sections, decay heat, fission yields) and material-input parameters. Sampler generates the uncertainty in any result generated by any computational sequence through statistical means by repeating numerous passes through the computational sequence, each with a randomly perturbed sample of the requested uncertain quantities.

ORNL implemented nuclear-covariance data generated by the XSUSA sampling code into Sampler (Bostelmann et al. 2016a). XSUSA was developed by the Gesellschaft für Anlagen und Reaktorsicherheit (GRS). The typical approach is to assume that the MG probability density functions are multivariate normal distributions, which are completely defined by the expected values and covariance matrices for the data. An XSUSA statistical sample consists of a full set of perturbed, infinitely dilute MG data for all groups, reactions, and materials.

The SCALE MG covariance data are given as relative values of the infinitely dilute cross-sections, so a random perturbation sample for cross-section  $\sigma_{x,g}(\infty)$  corresponds to  $\frac{\Delta\sigma_{x,g}(\infty)}{\sigma_{x,g}(\infty)}$ . XSUSA converts these values to a set of multiplicative perturbation factors,  $Q_{x,g}$ , which are applied to the reference data to obtain the altered values in the following equations:

$$\sigma'_{x,g} = Q_{x,g} \sigma_{x,g} \quad (3-2)$$

$$Q_{x,g} = 1 + \frac{\Delta\sigma_{x,g}(\infty)}{\sigma_{x,g}(\infty)} \quad (3-3)$$

(Note that this representation is simplified for this discussion; the XSUSA/Sampler perturbation factors also take into account correlations between cross sections. More detail can be obtained in the Sampler section of the SCALE manual [Rearden et al. 2016]). The XSUSA data set in Sampler is currently limited to 1,000  $Q_{x,g}$  factors for a subset of the most important reaction pairs. Two examples of the  $Q_{x,g}$  factors are shown in Figure 3-6 for the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  (left) and  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  (right) nuclear reaction pairs. Each of the plots contains 56,000 points, consisting of 1,000 Q-factors for each of the 56 covariance groups. The 56-groups are represented by 56 colours in the plots (not all of them visible at this size). It can be seen that the Q-factors are not normalized to 1.0, but all samples cluster around a mean value of 1.0 for each covariance group.

The two nuclear reaction sample sets vary significantly: the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  Q-factors are sampled between 0.0-2.0 with standard deviations of up to 40% in some groups (Figure 3-7), compared to the much smaller range and standard deviations for  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  (0.987-1.013 and less than 0.40%, respectively). The relative standard deviation ( $\sigma$ ) of a number of samples,  $N_s$ , can be computed using the sample mean  $\mu$  as the square root of the sample variance,  $var(R)$ , defined for any response,  $R$ , as:

$$\sigma = \frac{\sqrt{var(R)}}{R} \quad (3-4)$$

where

$$var(R) = \frac{\sum_{i=1}^{N_s} (R_i - \mu)^2}{N_s - 1} \quad (3-5)$$

It should be noted that this definition assumes that the sample distribution of the 1,000 FOMs (e.g. eigenvalues) is a normal distribution. As part of the sensitivity assessment, various statistical tests can be performed to confirm the applicability of this assumption, and usually more than one “normality test” are checked for conformance. This is an important element in statistical studies in which a smaller number of samples are taken (e.g. less than 100), but with a sample set of 1,000 calculations, this normality assumption is usually satisfied in the case of cross-section input uncertainties.

In the general RAVEN formulation, an interface is necessary to utilize RAVEN with an external code. Rouxelin (2019) developed and implemented a PHISICS interface to perturb the neutron cross-sections, the nuclide number densities, the decay constants, the fission yields, the energy emitted per fission and the energy emitted per decay. However, this RAVEN/PHISICS interface was not used in this work because RAVEN was not used to perturb the cross-section data - Sampler already provided this capability.

Since the XSUSA-derived  $Q_{x,g}$  factors in Equation (3-3) are available through the use of utility codes in the SCALE package, RAVEN could access the perturbed vector of all  $Q_{x,g}$  factors for each of the 1,000 entries in the Sampler data base. This allows RAVEN to determine sensitivity coefficients for the various cross-section reactions to the eigenvalue using the existing “PointSet” approach. RAVEN is also used in Section 7.5 for the creation of the perturbed RELAP5-3D input data and calculation of the Exercise IV-1 thermal fluid sensitivity coefficients, and for the U/SA of the coupled core Exercises III-1(Section 8.1.1) and IV-2 (Section 8.2). More detail is provided in each of these sections on the specific U/SA schemes used.

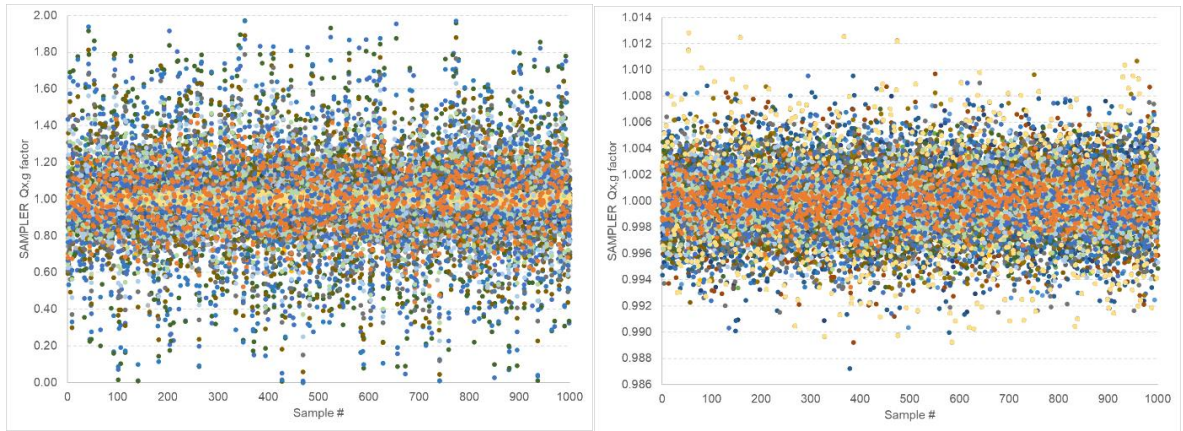


Figure 3-6. Sampler  $Q_{x,g}$  factors for  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  (left) and  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  (right) reactions.

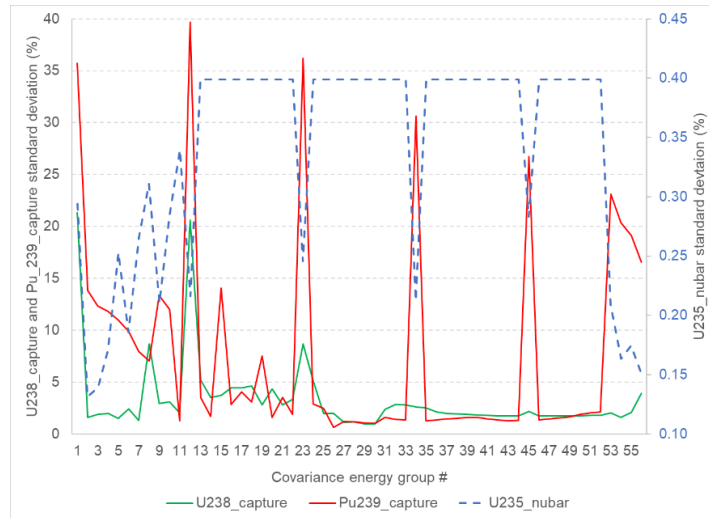


Figure 3-7. Comparison of the standard deviation (%) for 1,000 Sampler  $Q_{x,g}$  factors for the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$ ,  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$ , and  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  (right) reactions as a function of covariance energy group.

## 4. CROSS-SECTION UNCERTAINTY AND SENSITIVITY ANALYSIS OF THE VHTRC EXPERIMENT

*“No amount of experimentation can ever prove me right; a single experiment can prove me wrong.”*

Albert Einstein.

In this chapter, the statistical U/SA methodology is applied to a series of temperature-dependent criticality data measured at the experimental VHTRC facility as a partial validation of the sequence utilized for the MHTGR-350 design in Chapters 5-8. The VHTRC data set is valuable, not only for the validation of HTGR best-estimate criticality predictions, kinetic data, and temperature coefficients, but also for U/SA validation because an extensive effort has been included in the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhEP) to characterize individual and integral uncertainties. The uncertainty and sensitivity contributors for two critical core configurations at five temperatures are compared using the TSUNAMI, Sampler and PHISICS/RAVEN sequences. The predicted CE and MG uncertainty data obtained are also compared with the experimental uncertainties.

It is important to note that the aim of this chapter is not an exhaustive analysis of all possible sources of epistemic and aleatory uncertainties but, is limited to the uncertainty assessment of cross-section uncertainties and a comparison with measured<sup>12</sup> uncertainty data. Because cross-section uncertainties are only a component of the total calculation uncertainties, a definitive statement cannot be obtained on how well the simulation codes used in this work perform in predicting total uncertainties. The aim of a *complete* U/SA “validation” of the SCALE and PHISICS/RAVEN tool sets can therefore not be achieved by including only the cross-section uncertainties component, but a *partial* validation of the code sequence against one of the few sources of HTGR<sup>13</sup> measured uncertainty data is a valuable contribution.

It should also be stressed that although the VHTRC experiment includes measured data at various temperature points, the experimental setup is isothermal and without any coolant flow, and a RELAP5-3D model is consequently not required. The RELAP5-3D model used for the MHTGR-350 simulations reported in Chapter 5-8 can therefore not be validated using the VHTRC data set.

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<sup>12</sup> Caution is required in the interpretation of “measured” uncertainties because the final “measured” uncertainties contain calculated components as well (see Section 4.2 for detail).

<sup>13</sup> Although the VHTRC is representative of the typical HTGR spectrum—even if very low-enriched fuel was used—the experiment was not performed at prototypical temperatures. The highest temperature measured was only 200°C because the focus of the VHTRC was on reactor physics data.

## 4.1 Very High Temperature Reactor Critical Assembly Description

The VHTRC was a prismatic graphite-moderated single-block assembly located at the JAEA Tokai Research and Development Center in Japan. It first achieved criticality in May 1985 and was constructed to validate the neutronic design of the HTTR. Data generated by the VHTRC criticality measurements at several temperature points has been evaluated and included in the OECD/NEA IRPhEP (OECD/NEA 2006b) as a validation benchmark experiment for LEU graphite-moderated gas-cooled reactors. The VHTRC benchmark is especially valuable for uncertainty assessments because a significant effort was made to include uncertainty data for both the measured and calculated multiplication factors, as well as uncertainties on manufacturing and material composition parameters.

The VHTRC is a graphite-moderated thermal critical assembly that has a core loaded with pin-in-block fuel of LEU (i.e., to 2 and 4 wt%) and a graphite reflector (Figure 4-1). The assembly is a hexagonal prism, 2.4 m across the flats and 2.4 m long. The assembly consists of two axially jointed hexagonal-prism half assemblies, one of which is fixed, and the other movable. The structures of the half assemblies are made of graphite blocks supported with steel frames. The shape of the inner graphite blocks is hexagonal, while the outermost blocks, which are located along the radial perimeter of the core, are trapezoidal to form a hexagonal assembly. The fuel block has 19 holes into which fuel rods, graphite rods, lumped burnable poison (LBP) simulation rods, etc., can be inserted according to the requirements of the experiment. Each fuel rod is paired with a solid-graphite rod to reach an axial length of 1,200 mm. The fuel rod consists of 20 fuel compacts, one graphite sheath, and two graphite end caps. The “B-2” and “B-4” annular fuel rods used two types of fuel compacts containing 2 and 4 wt% enriched uranium, respectively.

The fuel compact is made of coated fuel particles uniformly dispersed in a graphite matrix. In contrast to the other HTGR designs (e.g. PBMR-400, MHTGR-350), the coated fuel particles are bistructural isotropic (BISO) particles (i.e. two carbon layers surrounding a LEU-dioxide kernel). Each fuel compact contains an average of approximately 20,000 randomly distributed BISO fuel particles. More detail on the B-2 and B-4 fuel designs can be found in the IRHP reference.

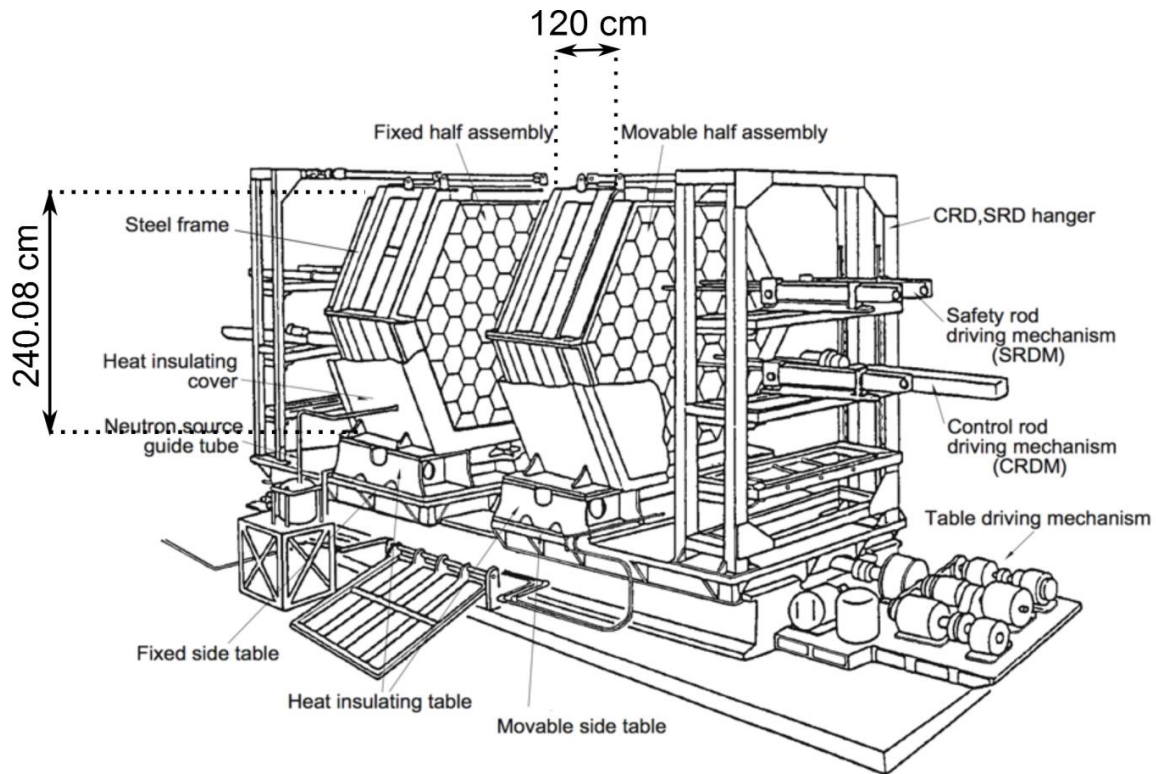


Figure 4-1. VHTRC assembly.

A series of experiments was performed with three different core-loading patterns: HP, HC-1, and HC-2. In the experiments using the HP core (shown in Figure 4-2), the assembly was first brought to critical state at room temperature (i.e., 25.5°C), and the critical point was determined using calibrated control rods. The HP core was then heated to 200°C using electric heaters. During the heating phase, the reactivity decrease due to the temperature rise was measured at four temperatures—71.2, 100.9, 150.5, and 199.6°C—by the pulsed neutron method. The critical points for the HC-1 (Figure 4-3) and HC-2 (Figure 4-4) cores were likewise determined at 8.0 and 200.3°C, respectively. Three critical configurations (for the HP, HC-1 and HC-2 cores) and four subcritical configurations (for the HP core only) were therefore obtained. However, due to the reactivity effects of loading irregularities, the measured eigenvalues were later corrected so that the VHTRC dataset contains four critical and three subcritical core states (Table 4-1).

The HP, HC-1, and HC-2 cores achieved different loading patterns by varying the number and type of fuel rods. The central region of all three configurations consisted of B-4-type fuel rods. The HP core has one graphite block that contains B-2-type fuel.

The  $C/^{235}\text{U}$  atomic ratio, which is an important factor in determining the spectral environment in the fuel region, is approximately 8,600 in the B-4-fuel center region. The HC-1 core is almost identical to the HP core, with only the B-2 fuel rods replaced by graphite rods (upper right fuel region of Figure 4-3). Core HC-2 contains an additional six B-2 fuel blocks compared to the HC-1 core, as well as a few additional B-4 fuel rods in the outer graphite blocks next to the central fuel blocks (Figure 4-4).

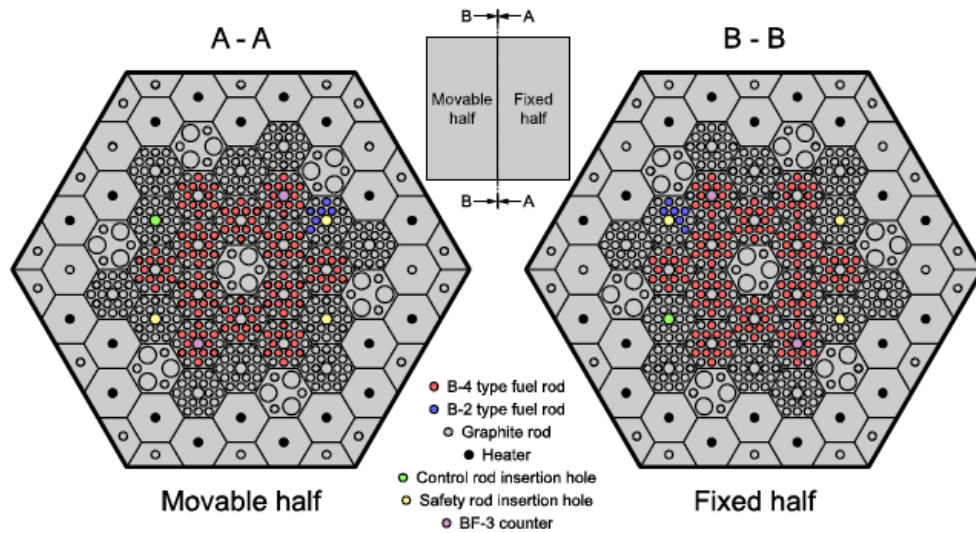


Figure 4-2. HP core-loading pattern.

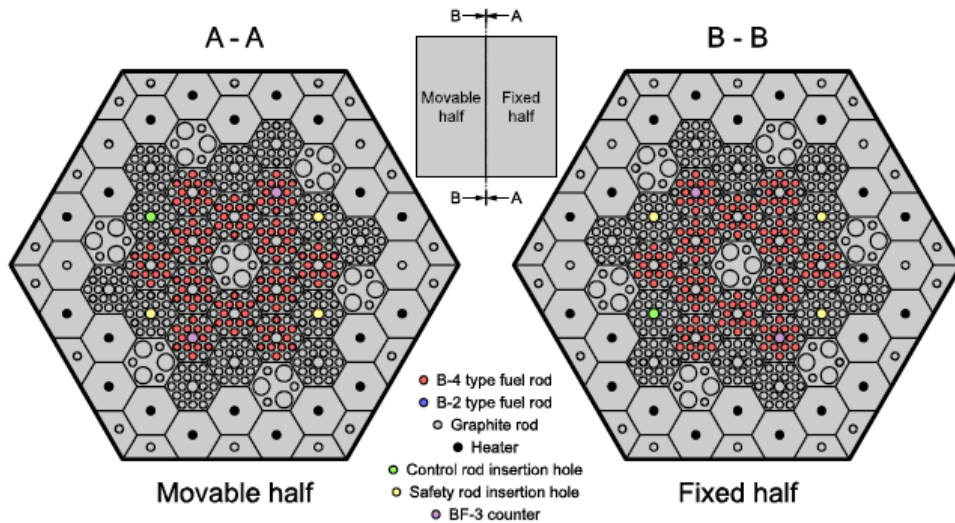


Figure 4-3. HC-1 core-loading pattern.

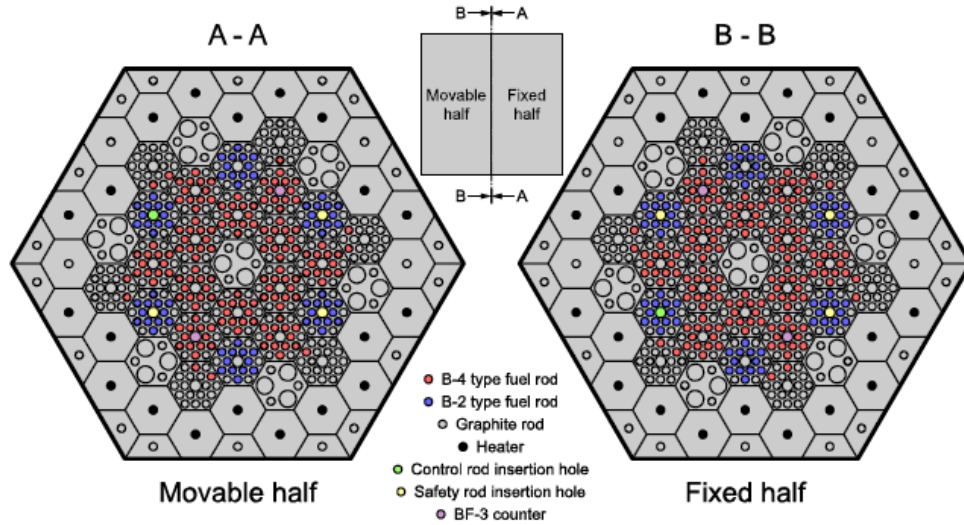


Figure 4-4. HC-2 core-loading pattern.

Table 4-1. Combined measured and calculated VHTRC eigenvalues and uncertainties for three core-loading patterns.

| Core | Temperature (°C) | $k_{\text{eff}}$      |
|------|------------------|-----------------------|
| HC-1 | 8.0              | $1.01218 \pm 0.00339$ |
| HP   | 25.5             | $1.01172 \pm 0.00323$ |
|      | 71.2             | $1.00480 \pm 0.00333$ |
|      | 100.9            | $0.99953 \pm 0.00350$ |
|      | 150.5            | $0.99074 \pm 0.00354$ |
|      | 199.6            | $0.98216 \pm 0.00368$ |
| HC-2 | 200.3            | $1.00895 \pm 0.00309$ |

## 4.2 Measured Results and Estimate of Uncertainties

The evaluation of the VHTRC set of experiments includes both the measured data and calculated estimates of various material, environmental, and experimental uncertainties. It is important to note that two main sets of data exist: the “raw” (uncorrected) measured data, and the VHTRC benchmark “corrected” data that attempt to take these various sources of uncertainties into account. The reactivity corrections were calculated with the JAEA Monte Carlo code MVP-II, and included corrections for the assembly gap, the positions of the control and safety rods, the replacement of the BF3 counters and heater elements by graphite, and the reactivity effect of moisture drying.

In addition to an evaluation of measurement uncertainties, the benchmark evaluators also assessed the uncertainties caused by material specifications (e.g. number of fuel particles, graphite density, impurities, etc.), by varying these parameters, one at a time<sup>14</sup>, in the MVP-II code (see Table 2.14 of the IRPhEP reference for more detail). The final “experimental” eigenvalues for the VHTRC benchmark obtained in this manner are listed in Table 4-1 (Table 2-15 of the IRPhEP reference) and consist of both measured and calculated components.

### 4.3 Codes and Models

As part of the INL contributions to the experiment validation phase of the IAEA HTGR UAM, three publications were produced. The first paper (Bostelmann et al. 2016b) compared the best-estimate (nominal) results against the experimental values using various KENO-VI and Serpent2 models and the 4<sup>th</sup> beta release of SCALE 6.2. A subsequent companion paper (Bostelmann and Strydom 2017) utilized refined versions of the same models and the first full release of SCALE 6.2.0. The statistical (simple random) sampling-based methodology was applied using both the GRS code XSUSA and the CE SCALE 6.2.0 Sampler/KENO-VI to assess uncertainties and derive sensitivity coefficients. The Sampler/KENO-VI results were also compared with the CE results obtained from the deterministic linear perturbation theory-based TSUNAMI module. (The XSUSA results included in the 2016 PHYSOR paper (Bostelmann et al. 2016c) were not included in the 2017 paper because it used the older ENDF/B-VII.0 cross-sections at the time).

Because the author was involved in these publications in the context of his contributions to the CRP, a summary of the results is included in Section 4.4 to allow a comparison with the current research. The Sampler/NEWT 252-group models developed by Rouxelin (2019) for his assessment of VHTRC manufacturing and material uncertainties are again utilized in this chapter for the RAVEN assessment of cross-section uncertainties and sensitivities to allow direct comparison between the two sets of U/SA results.

#### 4.3.1 General Process Flow

The RAVEN code is used to perform a statistical analysis of output uncertainties and sensitivities. An overview of the calculation process flow is provided in Figure 4-5.

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<sup>14</sup> The one-by-one variance approach followed by the benchmark team is simplistic and possibly too conservative. Table 4-1 is however listed as the formal benchmark eigenvalue set. Rouxelin (2019) seems to be the only author so far that expressed concern about the lack of a rigorous U/SA approach followed – a concern noted here as well.

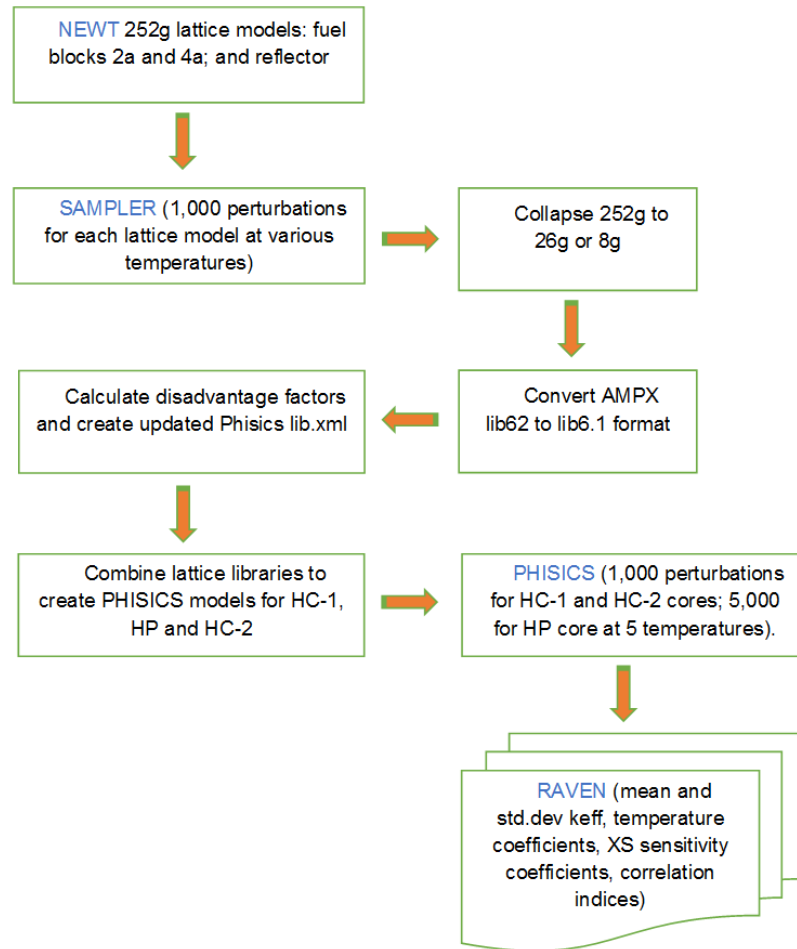


Figure 4-5. VHTRC calculation process flow.

The Sampler sequence is used to create a set of 1,000 NEWT lattice models for each lattice/reflector type, which is subsequently used for the full-core VHTRC PHISICS simulations. These models used the 252-group scheme. In the final step, RAVEN is applied to determine the statistical parameters of interest.

In contrast to Rouxelin's approach, where RAVEN was used as the active driver for the RAVEN/SCALE/PHISICS interface, RAVEN was used in the current sequence to perform *only* the statistical analysis on a Sampler/NEWT/PHISICS sequence via the existing RAVEN "PointSet" approach. The most-important difference is that in Rouxelin's scheme, RAVEN generated the perturbed *material*-data input uncertainties, compared to the current scheme where Sampler was used to generate the perturbed *cross-section* libraries used in the NEWT-to-PHISICS propagation. In the 5<sup>th</sup> step of the process flow shown in Figure 4-5, NEWT produces microscopic self-shielded, collapsed cross-section libraries in 8, 26 or 245-energy groups (file ft30f001).

These libraries do not include the flux disadvantage factors described in Equation (3-1) in Section 3.2.2, and therefore require further corrections to account for spatial self-shielding in a material after the homogenization process. Rouxelin (2019) developed a stand-alone Python procedure to parse the 252-group scalar fluxes relative to each mixture defined in NEWT and produce corrected few-group homogenized microscopic AMPX cross-sections for use in PHISICS.

#### 4.3.2 Serpent2, KENO-VI, TSUNAMI and Sampler Models

The models developed by the author and Bostelmann for the 2017 study (Bostelmann and Strydom 2017) are based on the final IRPhEP benchmark specifications. As basis for the subsequent uncertainty and sensitivity analyses, nominal criticality calculations are performed with the Monte Carlo codes KENO-VI and Serpent2. The Serpent2 models includes the explicit stochastic modeling of randomly distributed particles in the fuel compacts (Figure 4-6), but to allow comparisons with KENO-VI results, the Serpent2 particles were also included in a regular lattice model variant. The Serpent2 models utilized 500,000 neutrons per cycle and a total of 300 active cycles to assure convergence of the multiplication factor, with the first 40 cycles skipped to assure convergence of the Shannon entropy of the fission source distribution.

The KENO-VI CE VHTRC models are identical to the lattice variants of the Serpent2 models. In this case, 100,000 neutrons in 1,000 active cycles and 100 initially skipped cycles were used. For the CE KENO-VI calculation, the fuel compacts are modeled as regular particle lattices to represent the double-heterogeneity of the VHTRC system (Figure 4-7).

Problem-dependent cross-sections for the MG KENO-VI and NEWT calculations are determined during the initial self-shielding calculation, as described in Section 4.3 of the MHTGR-350 discussion. For 2016 and 2017 VHTRC studies, both the ENDF/B-VII.0 and ENDF/B-VII.1 libraries were used, but the latest calculations performed by the author and Rouxelin only utilized the ENDF/B-VII.1 library.

For the CE TSUNAMI calculations with CLUTCH, the location-dependent weighting function utilized a grid for the VHTRC that divided each fuel unit cell into two or four in the horizontal axis (Figure 4-8).

A total of 10 latent generations were used in 3,000 inactive generations with 50,000 neutrons per generation to ensure convergence of the weighting function; in total 50,000 neutrons in 6,000 active and 3,000 inactive cycles were calculated. The axial dimensions of the models are indicated in Figure 4-9.

The Sampler perturbations utilized the same KENO-VI and NEWT models developed for the nominal calculations and were performed in parallel on the INL computational cluster in sets of 1,000, representing the HC-1, HC-2 and HP core configurations and temperatures.

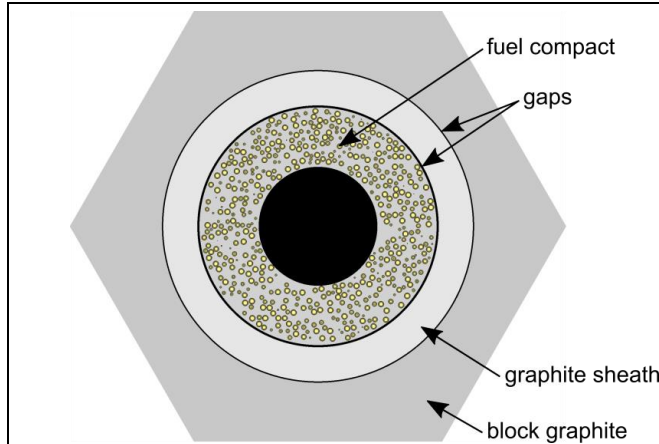


Figure 4-6. Cross sectional view of fuel unit cell with randomly distributed particles (Serpent2 model) - (Bostelmann & Strydom, 2017).

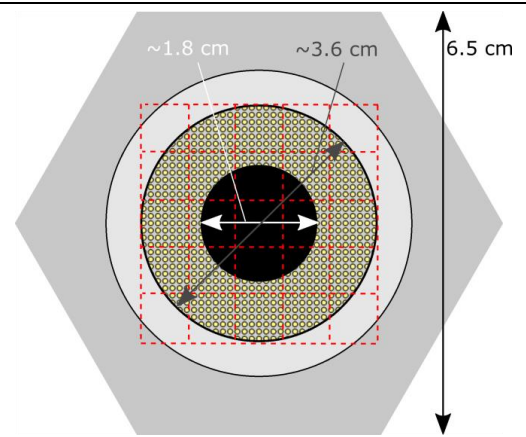


Figure 4-7. Cross sectional view of a fuel unit or compact cell. Dashed lines indicate the grid for the CE TSUNAMI fuel compact and unit cell models.

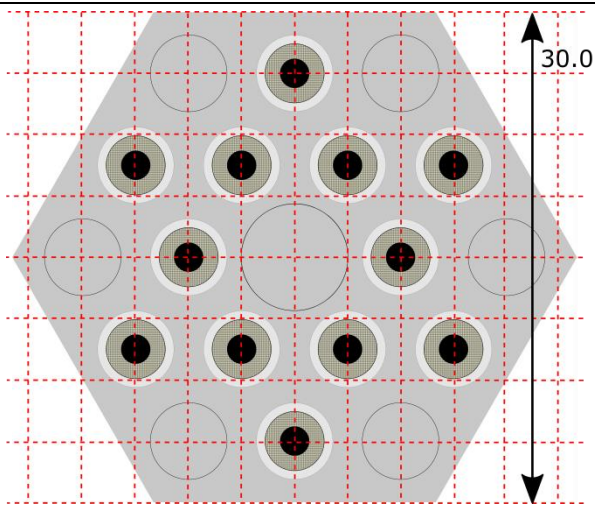


Figure 4-8: Cross sectional view of a fuel block (KENO-VI model). Dashed lines indicate the grid for the CE TSUNAMI fuel block and full core models.

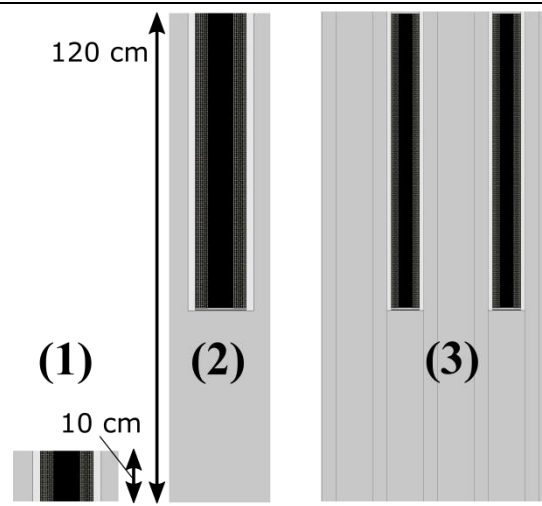


Figure 4-9: Axial cut of (1) a fuel compact cell, (2) a fuel unit cell, and (3) a fuel block (KENO-VI model) - (Bostelmann & Strydom, 2017).

For the U/SA of the VHTRC, the TSUNAMI and Sampler modules of SCALE 6.2.0 were used with the CE and MG models, respectively. RAVEN used as statistical processor for the NEWT/PHISICS/Sampler sequence because Sampler does not provide sensitivity information yet.

In addition, the CLUTCH method implemented in the SCALE/TSUNAMI module was used to obtain the reference CE sensitivity coefficients. By collapsing the determined sensitivity coefficients with available covariance data, nuclear data eigenvalue uncertainties are obtained. CE TSUNAMI is applied with both ENDF/B-VII.0 and ENDF/B-VII.1 data. Because the CE Monte Carlo method is applied, the double-heterogeneity of the HTGR model is considered by specifying a regular particle lattice as described for KENO-VI in CE mode. A summary of the codes, libraries and models utilized for the VHTRC assessment is presented in Table 4-2.

Table 4-2. Overview of the applied codes and nuclear data libraries for the VHTRC calculations.

| Code                                        | ENDF/B-VII.0 data                 | ENDF/B-VII.1 data                       |
|---------------------------------------------|-----------------------------------|-----------------------------------------|
| <i>Nominal (best-estimate) calculations</i> |                                   |                                         |
| Serpent 2.1.26                              | CE (random particle distribution) | CE (random particle distribution)       |
| Serpent 2.1.26                              | CE (particle lattice)             | CE (particle lattice)                   |
| SCALE 6.1.2/KENO-VI                         | 238g                              | -                                       |
| SCALE 6.2/KENO-VI                           | 238g                              | 252g                                    |
| SCALE 6.2/KENO-VI                           | CE (particle lattice)             | CE (particle lattice)                   |
| SCALE 6.2/NEWT                              | -                                 | 252g                                    |
| <i>Uncertainty assessment</i>               |                                   |                                         |
| KENO-VI/TSUNAMI                             | -                                 | CE (particle lattice)                   |
| KENO-VI/Sampler                             | 238g                              | 252g                                    |
| NEWT/PHISICS/Sampler/RAVEN                  | -                                 | 252g (NEWT); 245g, 26g and 8g (PHISICS) |
| <i>Sensitivity assessment</i>               |                                   |                                         |
| KENO-VI/TSUNAMI                             | 238g                              | 252g, CE                                |
| KENO-VI/Sampler/XSUSA                       | 238g                              | -                                       |
| NEWT/PHISICS/Sampler/RAVEN                  | -                                 | 252g                                    |

### 4.3.3 NEWT & PHISICS Models

Rouxelin defined three NEWT lattice cells to simulate the HC1, HC2, and HP core configurations in PHISICS (Rouxelin 2019). The VHTRC core consist of mostly 4.0 wt% enriched blocks in the central rings of the core, and 2.0 wt% enriched blocks in the outer fuel rings. A lattice cell generates two or three sets of cross-sections, depending on the core configuration: the central block in Figure 4-10 provides the 4.0 wt% enriched fuel block's cross-sections, the (green) graphite block provides the reflector cross-sections, and

the right fuel block (Figure 4-10) models the 2.0 –enriched blocks found in the VHTRC core. The lattice cell VHTRC HC-1 (Figure 4-10, left) is executed twice in NEWT; once for the fuel and once for the reflector. The PHISICS model of the VHTRC should consist of five rings (Figure 4-2), but because PHISICS cannot model the real geometry of the VHTRC (the half-blocks lead to a trapezoidal geometry), the model excludes a section of the absorber blanket surrounding the core and assumes vacuum boundary conditions, as shown in Figure 4-11. The PHISICS model therefore neglects back-scattering from the blanket and the environment, which could lead to a slight underestimation of the eigenvalue. In addition, the PHISICS model does not include the control rod in the (non-active core) upper reflector region because control-rod details were not provided in the specifications. The electric heater channels, control-rod insertion holes, and the  $\text{BF}_3$  counter slots were also filled with graphite.

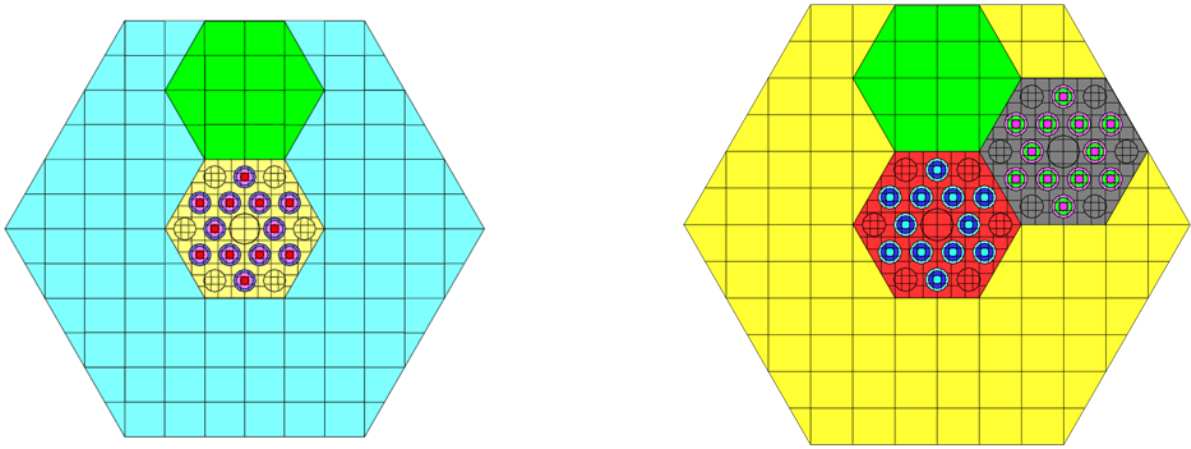


Figure 4-10. Left: VHTRC lattice model for the HC-1 core. Right: the HP core (Rouxelin 2019).<sup>19</sup>

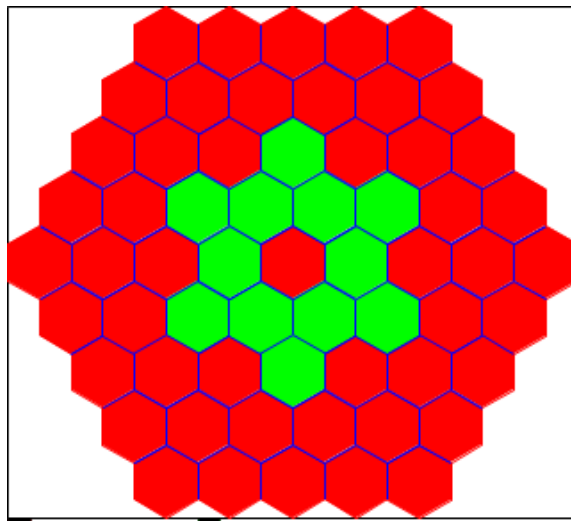


Figure 4-11. VHTRC HC-1 core shape in PHISICS (Rouxelin 2019).<sup>19</sup>

## 4.4 Results

### 4.4.1 Uncertainty Results

The use of the older ENDF/B-VII.0 library lead to significant overestimations of the VHTRC eigenvalues, mostly attributed to a change in the capture cross-section of carbon in the ENDF/B-VII.1 library. A comparison reported in the 2017 study by Bostelmann and Strydom found differences varying between the libraries of 1.2–1.4% for both the Serpent2 and SCALE models. It can be seen in Figure 4-12 that the nominal ENDF/B-VII.1 results mostly match the measured VHTRC data within the experimental uncertainty band. Based on this finding, only the ENDF/B-VII.1 library was used in the generation of the PHISICS results.

In addition, the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  uncertainty in the thermal-energy range was increased from 0.311% in the ENDF/B-VII.0 library to 0.385% in the ENDF/B-VII.1 library (Marshall et al. 2015). In the VHTRC models, this change led to an increase in the eigenvalue uncertainty from 0.57% to 0.66% (Table 4-3). Since the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  uncertainty is the most-important contributor to the total eigenvalue uncertainty (as shown later in Table 4-9), this change incorporated into ENDF/B-VII.1 is an important update to the covariance libraries that will influence the U/SA of most thermal uranium-fueled systems.

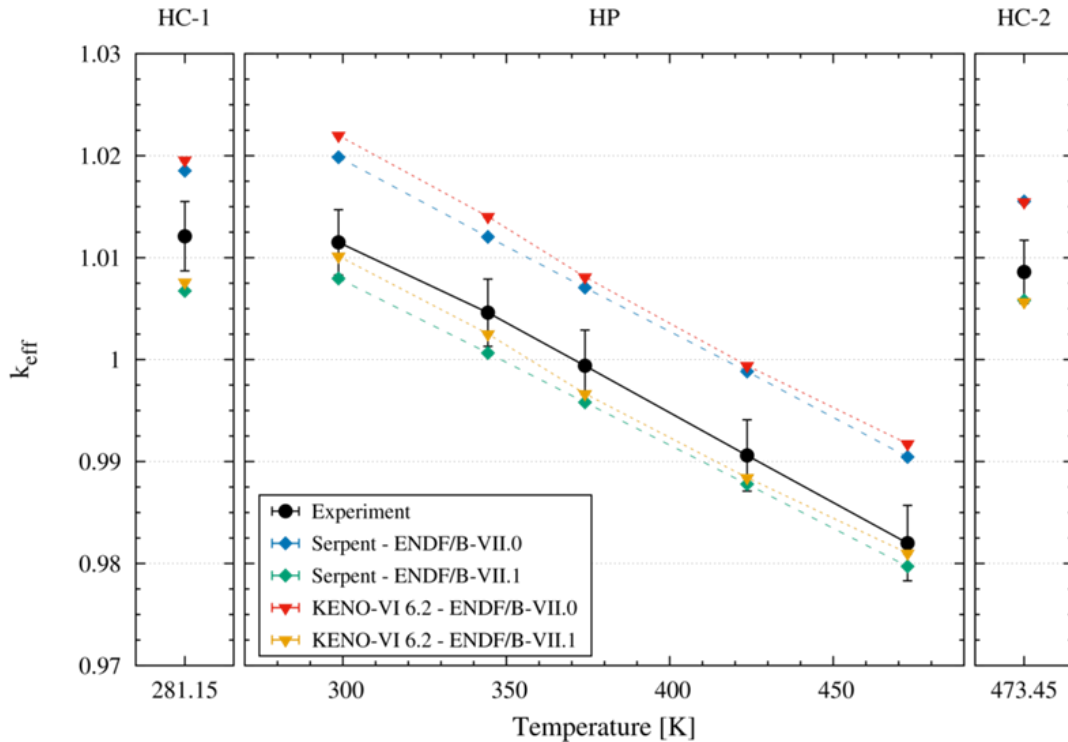


Figure 4-12. Comparison of the KENO-VI CE and Serpent2 CE solutions of the nominal VHTRC multiplication factors (Bostelmann and Strydom 2017)<sup>159</sup>

The VHTRC eigenvalues obtained for both the statistical (Sampler) and deterministic (TSUNAMI) options available in SCALE are presented in Table 4-3. Identical KENO-VI models were used for both sets of calculations; in the case of Sampler a total of 1,000 cross-section perturbed libraries were used for each core state and temperature point. In this table, the KENO-VI values are the population mean  $k_{\text{eff}} \pm \sigma_s$ , with  $\sigma_s$  the Monte Carlo statistical uncertainty, and  $\sigma_{\text{tsunami}}$  the deterministic uncertainty determined by the GPT method in TSUNAMI. For the Sampler sequence, the mean  $k_{\text{eff}}$  is calculated as the mean value of the 1,000 KENO-VI VHTRC samples, with  $\sigma_s$  the 95% confidence intervals on the mean values of the 1,000 Monte Carlo statistical uncertainties for this set (see Section 3.2.2.2). The  $\sigma_{\text{sampler } k_{\text{eff}}}$  value is the one sigma standard deviation of the 1,000 sample population in %, i.e.  $(100 \times \sigma_{\text{sampler}}/\text{mean})$ .

The KENO-VI mean multigroup eigenvalues are in general a few hundred pcm lower than the mean KENO-VI CE results, but for both ENDF/B library sets the Sampler uncertainties are very close to TSUNAMI uncertainties, as shown in Table 4-3. The conclusion from this data set is that although differences are observed between the CE and MG nominal and mean eigenvalues, the ENDF/B.VII.1 eigenvalue uncertainty is consistently estimated as 0.66%.

Table 4-3. Comparison of the VHTRC ENDF/B-VII.0 and ENDF/B-VII.1 KENO-VI and TSUNAMI uncertainty results.

| Core | T<br>(K) | ENDF/B-VII.0                         |                                  |                                      |                                  | ENDF/B-VII.1                         |                                   |                                      |                                  |
|------|----------|--------------------------------------|----------------------------------|--------------------------------------|----------------------------------|--------------------------------------|-----------------------------------|--------------------------------------|----------------------------------|
|      |          | 238g KENO-VI/Sampler                 |                                  | CE TSUNAMI                           |                                  | 252g KENO-VI/Sampler                 |                                   | CE TSUNAMI                           |                                  |
|      |          | $k_{\text{eff}}$ mean $\pm \sigma_s$ | $\sigma_{\text{sampler}}$<br>(%) | $k_{\text{eff}}$ mean $\pm \sigma_s$ | $\sigma_{\text{tsunami}}$<br>(%) | $k_{\text{eff}}$ mean $\pm \sigma_s$ | $\sigma_{\text{sample}}$<br>r (%) | $k_{\text{eff}}$ mean $\pm \sigma_s$ | $\sigma_{\text{tsunami}}$<br>(%) |
| HC-1 | 281      | 1. 02079 (36) <sup>15</sup>          | 0.576                            | 1.01954 (5)                          | 0.587                            | 1.00730 (41)                         | 0.661                             | 1.00768 (5)                          | 0.669                            |
| HP   | 298      | 1.02136 (36)                         | 0.569                            | 1.02204 (5)                          | 0.592                            | 1.00805 (41)                         | 0.664                             | 1.01007 (5)                          | 0.664                            |
|      | 344      | 1.01319 (36)                         | 0.566                            | 1.01405 (5)                          | 0.585                            | 0.99922 (41)                         | 0.662                             | 1.00236 (5)                          | 0.658                            |
|      | 374      | 1.00799 (35)                         | 0.565                            | 1.00802 (5)                          | 0.591                            | 0.99369 (41)                         | 0.662                             | 0.99653 (5)                          | 0.667                            |
|      | 423      | 0.99959 (35)                         | 0.563                            | 0.99925 (5)                          | 0.603                            | 0.98545 (40)                         | 0.661                             | 0.98830 (5)                          | 0.662                            |
|      | 473      | 0.99153 (35)                         | 0.563                            | 0.99165 (5)                          | 0.591                            | 0.97822 (40)                         | 0.661                             | 0.98097 (5)                          | 0.656                            |
| HC-2 | 473      | 1.01540 (35)                         | 0.555                            | 1.01542 (5)                          | 0.588                            | 1.00315 (41)                         | 0.653                             | -                                    | -                                |

<sup>15</sup> The notation of  $1.02079 \pm 0.00036 = 1.02079$  (36) is used.

The 26-group PHISICS nominal, mean, 95<sup>th</sup> percentile, and standard-deviation eigenvalues are indicated in Table 4-4, together with several other standard statistical indicators. The absolute (pcm) and relative (%) differences between the calculated and experimental results are also included in this table. Regardless of the VHTRC-core loading and temperature, the uncertainties in the cross-sections lead to an uncertainty of 0.64% in the PHISICS eigenvalue. This is very well matched with the Sampler/KENO-VI and TSUNAMI model predictions of 0.66% (Table 4-5).

Because the NEWT and KENO-VI models were independently developed, and both statistical and deterministic methods were used, this provides a very good verification basis for the use of the Sampler/NEWT/PHISICS sequence. The relative difference between the calculated PHISICS and experimental eigenvalues ranges from -0.46 to 0.97%.

Table 4-4. RAVEN statistical detail of the 26-group VHTRC NEWT/PHISICS/Sampler results.

| Indicator                  | HC-1    | HP      |         |         |         |         | HC-2     |
|----------------------------|---------|---------|---------|---------|---------|---------|----------|
|                            | 281     | 298     | 344     | 374     | 423     | 473     | 473      |
| nominal keff               | 1.02035 | 1.02217 | 1.01115 | 1.00604 | 0.99843 | 0.99079 | 1.00476  |
| mean keff                  | 1.02033 | 1.02149 | 1.01052 | 1.00544 | 0.99788 | 0.99029 | 1.00430  |
| sigma (abs)                | 0.00651 | 0.00654 | 0.00645 | 0.00642 | 0.00637 | 0.00631 | 0.00636  |
| sigma (%)                  | 0.638   | 0.640   | 0.638   | 0.639   | 0.638   | 0.637   | 0.633    |
| 95th percentile            | 1.03121 | 1.03232 | 1.02105 | 1.01606 | 1.00858 | 1.00096 | 1.01465  |
| Experimental Data          |         |         |         |         |         |         |          |
| experiment keff            | 1.01218 | 1.01172 | 1.0048  | 0.99953 | 0.99074 | 0.98216 | 1.00895  |
| sigma (abs)                | 0.00339 | 0.00323 | 0.00333 | 0.00350 | 0.00354 | 0.00368 | 0.00309  |
| sigma (%)                  | 0.335   | 0.319   | 0.331   | 0.350   | 0.357   | 0.375   | 0.306    |
| (CE)/E (abs) <sup>16</sup> | 0.00806 | 0.00966 | 0.00569 | 0.00592 | 0.00721 | 0.00828 | -0.00461 |
| (CE)/E (%)                 | 0.81    | 0.97    | 0.57    | 0.59    | 0.72    | 0.83    | -0.46    |

<sup>16</sup> The relative difference between calculation and experiment in absolute and % units: (Calculation-Experiment)/Calculation

Table 4-5. Comparison of the KENO-VI, TSUNAMI and PHISICS uncertainty results.<sup>17</sup>

| Core | T (K) | Experiment |              | ENDF/B-VII.1                  |                            |                     |                            |                               |                           |
|------|-------|------------|--------------|-------------------------------|----------------------------|---------------------|----------------------------|-------------------------------|---------------------------|
|      |       |            |              | 252g KENO-VI/Sampler          |                            | 26g PHISICS/Sampler |                            | CE TSUNAMI                    |                           |
|      |       | $k_{eff}$  | $\sigma$ (%) | $k_{eff}$ mean $\pm \sigma_s$ | $\sigma_{sample}$<br>r (%) | mean $k_{eff}$      | $\sigma_{sample}$<br>r (%) | $k_{eff}$ mean $\pm \sigma_s$ | $\sigma_{tsunami}$<br>(%) |
| HC-1 | 281   | 1.0122     | 0.335        | 1.00730 (41)                  | 0.661                      | 1.02033 (40)        | 0.638                      | 1.00768 (5)                   | 0.669                     |
| HP   | 298   | 1.0117     | 0.319        | 1.00805 (41)                  | 0.664                      | 1.02149 (41)        | 0.640                      | 1.01007 (5)                   | 0.664                     |
|      | 344   | 1.0048     | 0.331        | 0.99922 (41)                  | 0.662                      | 1.01052 (40)        | 0.638                      | 1.00236 (5)                   | 0.658                     |
|      | 374   | 0.9995     | 0.350        | 0.99369 (41)                  | 0.662                      | 1.00544 (40)        | 0.639                      | 0.99653 (5)                   | 0.667                     |
|      | 423   | 0.9907     | 0.357        | 0.98545(40)                   | 0.661                      | 0.99788 (39)        | 0.638                      | 0.98830 (5)                   | 0.662                     |
|      | 473   | 0.9822     | 0.375        | 0.97822 (40)                  | 0.661                      | 0.99029 (39)        | 0.637                      | 0.98097 (5)                   | 0.656                     |
| HC-2 | 473   | 1.009      | 0.306        | 1.00315 (41)                  | 0.653                      | 1.00429 (39)        | 0.633                      | -                             | -                         |

It is shown in Figure 4-13 that, for most cases, the PHISICS simulations agree with the experimental data within  $2\sigma$  of the experimental uncertainty. In general, the PHISICS models overestimate the eigenvalues, except for the HC-2 core loading, where an underprediction of 0.46% was calculated. This core contained the highest fuel loading and lowest carbon-to-uranium ratio, resulting in a slightly harder spectrum. However, a more-detailed investigation into local reaction rates and spectral indices would be required to identify the root cause of this change in the general overestimation trend.

<sup>17</sup> The CE TSUNAMI statistical Monte Carlo errors and the 252g KENO-VI and PHISICS Sampler 95% confidence intervals on the mean values are shown as  $\pm x$ .

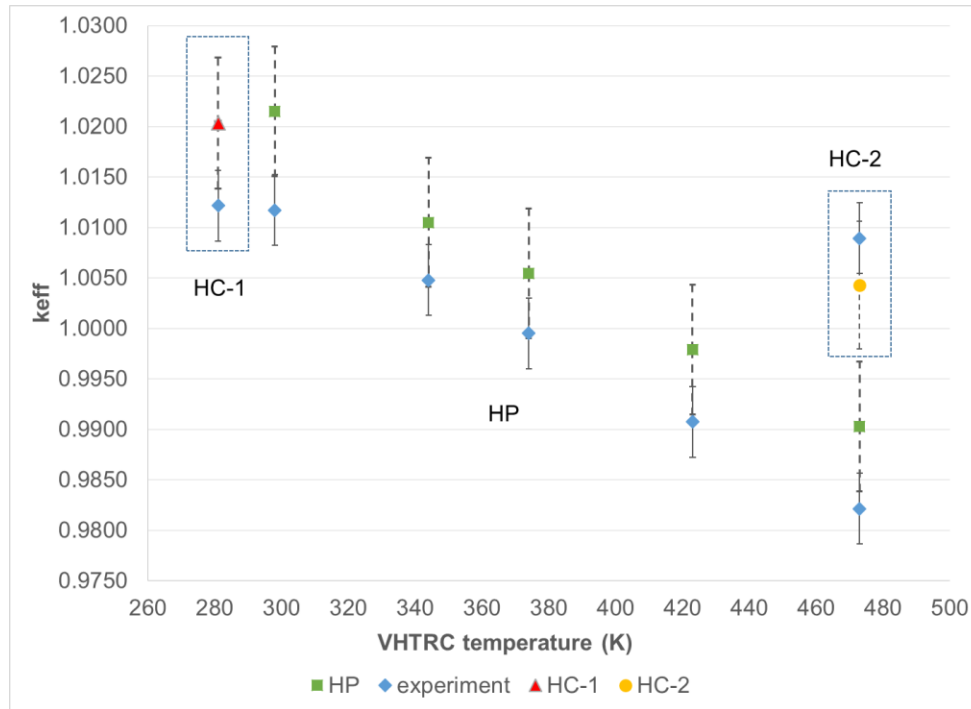


Figure 4-13. Comparison of VHTRC PHISICS and experimental results.

A summary of various uncertainty estimates is provided in Table 4-6. The uncertainties in the cross-section data resulted in PHISICS eigenvalue uncertainties that are significantly higher (631–654 pcm) than the experimental uncertainties (309–354 pcm). Rouxelin (2019) found that the impact of manufacturing uncertainties leads to eigenvalue uncertainties varying between 233–346 pcm. His RAVEN results provided an independent confirmation of the JAEA results obtained with the MVP-II code. The uncorrected “measured” experimental uncertainties are ten times smaller (31–56 pcm) than the uncertainty simulated with the MVP-II code.

Because the NEWT/PHISICS models and statistical methodology utilized by the author and Rouxelin are identical, the two uncertainty contributors can be compared directly. It therefore seems that cross-section uncertainties contribute significantly more than manufacturing uncertainties towards the uncertainty in the calculated VHTRC eigenvalues.

The contributions of each of these input uncertainties to the total calculation uncertainty can, however, only be assessed by combining all known input uncertainties in a consistent and simultaneous statistical-uncertainty assessment. This element was beyond the scope of the current work.

Table 4-6. VHTRC eigenvalue uncertainties: estimates of various contributions.

| Indicator                                     | HC-1    | HP      |         |         |         |         | HC-2    |
|-----------------------------------------------|---------|---------|---------|---------|---------|---------|---------|
|                                               | 281     | 298     | 344     | 374     | 423     | 473     | 473     |
| “Uncorrected” experiment<br>(IRPhEP)          | 0.00031 | 0.00030 | 0.00034 | 0.00041 | 0.00052 | 0.00065 | 0.00056 |
| “Corrected” MVP-II estimate<br>(IRPhEP)       | 0.00339 | 0.00323 | 0.00333 | 0.00350 | 0.00354 | 0.00368 | 0.00309 |
| Manufacturing uncertainties<br>(Rouxelin)     | 0.00318 | 0.00319 | 0.00330 | 0.00333 | 0.00339 | 0.00346 | 0.00233 |
| Cross-section uncertainties<br>(this section) | 0.00651 | 0.00654 | 0.00645 | 0.00642 | 0.00637 | 0.00631 | 0.00636 |

A comparison between the PHISICS/Sampler, KENO-VI/Sampler and experimental data is provided in Table 4-7 and Figure 4-14. In relative terms, the 252g KENO-VI data agrees better with the experimental data (0.36–0.58% difference) than the 26g PHISICS data (0.46–0.97%). The mean values of the two calculations vary between 0.11–1.33% (see the last column of Table 4-7), which is within the  $2\sigma$  experimental uncertainty margin. The differences between the KENO-VI and PHISICS results are mainly caused by the energy-group structure (252-group vs. 26-group), the transport solvers (Monte Carlo vs.  $S_3$  transport), and the 2D NEWT lattice cell and PHISICS model approximations (Section 4.3.3).

The impact on the U/SA results obtained with various energy-group structures has not yet been reported extensively in the literature. Rouxelin (2019) used RAVEN to compare the impact of manufacturing uncertainties on the VHTRC eigenvalue uncertainties using a 6- and 56-group structure. He found that the output uncertainty in the eigenvalue tends to be about 10% lower for the 56-group simulations. A similar reduction in the uncertainties is not seen for the cross-section uncertainties in Table 4-8, where a comparison of the 8- and 26-group PHISICS results for three of the core cases is shown. The 8- and 26-group structures produced very closely matched  $1\sigma$  eigenvalue uncertainty values (0.63%) when the cross-section covariances are considered. The mean 8- and 26-group eigenvalues differ by 0.89–1.11% for the HC-1, HP and HC-2 cores, which is significant for best-estimate core eigenvalues, where differences of less than ~0.3% are achievable.

Table 4-7. Comparison of KENO-VI, PHISICS and experimental results for the VHTRC.

| Core | T (K)  | Experiment | 252g KENO-VI/Sampler | (C-E)/E (%) | 252g PHISICS/Sampler | (C-E)/E (%) | (K-P)/K (%) <sup>18</sup> |
|------|--------|------------|----------------------|-------------|----------------------|-------------|---------------------------|
| HC-1 | 281.15 | 1.01218    | 1.00730              | -0.48       | 1.02033              | 0.81        | -1.29                     |
| HP   | 298.65 | 1.01172    | 1.00805              | -0.36       | 1.02149              | 0.97        | -1.33                     |
|      | 344.35 | 1.00480    | 0.99922              | -0.56       | 1.01052              | 0.57        | -1.13                     |
|      | 374.05 | 0.99953    | 0.99369              | -0.58       | 1.00544              | 0.59        | -1.18                     |
|      | 423.65 | 0.99074    | 0.98545              | -0.53       | 0.99788              | 0.72        | -1.26                     |
|      | 472.75 | 0.98216    | 0.97822              | -0.40       | 0.99029              | 0.83        | -1.23                     |
| HC-2 | 473.45 | 1.00895    | 1.00315              | -0.57       | 1.00429              | -0.46       | -0.11                     |

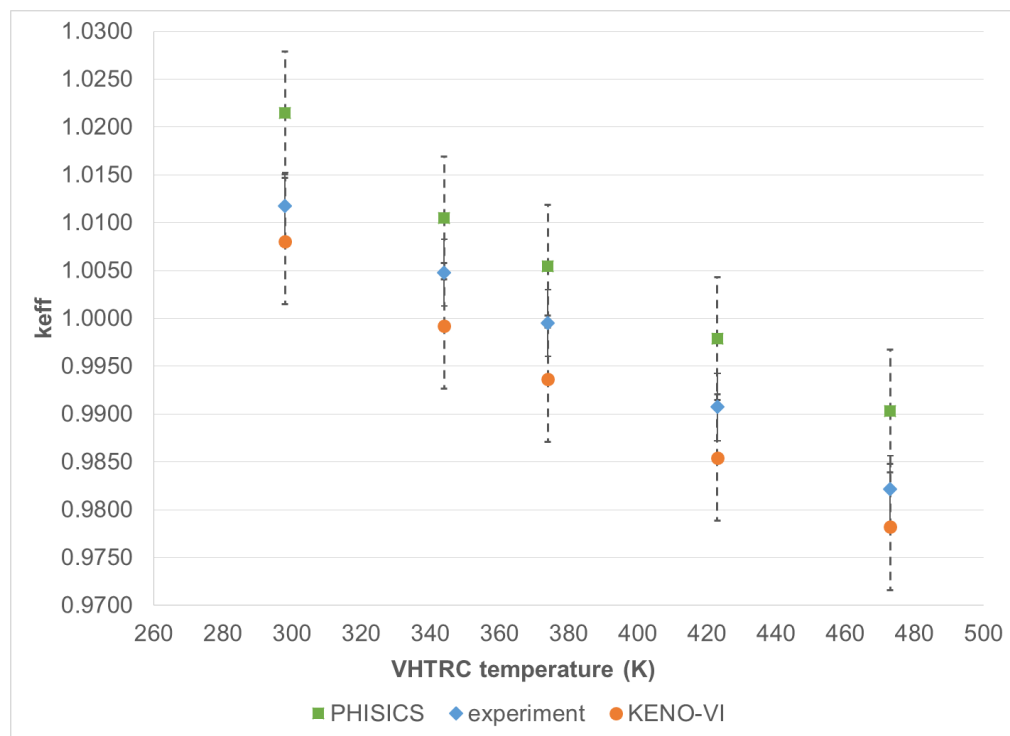


Figure 4-14. Comparison of VHTRC PHISICS, KENO-VI and experimental data for the HP core load.

<sup>18</sup> Relative difference between the mean KENO-VI and PHISICS eigenvalues:  $(\mathbf{K}_{\text{eno-IV}} - \mathbf{P}_{\text{HISICS}})/\mathbf{P}_{\text{HISICS}}$

In terms of the performance against the HC-1 and HP experimental values, the 8-group eigenvalues are 1.92% higher than the experimental values, compared to 0.83% for the 26-group results. The 26-group library would therefore be the most accurate option to use for the *nominal* (best-estimate) VHTRC analysis, but for the assessment of cross-section uncertainties, the 8-group structure produces identical eigenvalue uncertainties to the 26-group models. The 8-group structure can therefore be used for transient U/SA studies where minimizing calculation runs times is desirable, and nominal values are not the focus, e.g. as used in the transient MHTGR-350 calculations reported in Chapter 8.

Table 4-8. Comparison of 8- and 26-group VHTRC PHYSICS/Sampler eigenvalue results.

| Indicator        | HC-1    |         | HP      |         | HC-2    |         |
|------------------|---------|---------|---------|---------|---------|---------|
|                  | 281_8g  | 281_26g | 473_8g  | 473_26g | 473_8g  | 473_26g |
| experiment       | 1.01218 | 1.01218 | 0.98216 | 0.98216 | 1.00895 | 1.00895 |
| mean keff        | 1.03168 | 1.02033 | 1.00086 | 0.99029 | 1.01324 | 1.00430 |
| (8g-26g)/26g (%) | 1.112   | -       | 1.067   | -       | 0.891   | -       |
| (C-E)/E (%)      | 1.926   | 0.806   | 1.904   | 0.828   | 0.425   | -0.461  |
| sigma (abs)      | 0.00653 | 0.00651 | 0.00630 | 0.00631 | 0.00633 | 0.00636 |
| sigma (%)        | 0.633   | 0.638   | 0.630   | 0.637   | 0.625   | 0.633   |

#### 4.4.2 Sensitivity Results

For the sensitivity assessment of the VHTRC, two sets of results are available based on the SCALE/TSUNAMI (deterministic) and Sampler/RAVEN (statistical) sequences. The work performed in 2017 by Bostelmann and Strydom used the CE TSUNAMI module of SCALE 6.2.0 to calculate various indicators of interest, e.g. energy-integrated sensitivity coefficients, nuclide-reaction pair contributors to the overall eigenvalue uncertainty, etc., based on the 252- or 56-group covariance libraries. The deterministic TSUNAMI module provides energy-, region- and mixture-integrated sensitivity coefficients calculated using first-order perturbation theory. These data are presented in Table 4-9 for the VHTRC data set, where it is shown that the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ , C-graphite (n,n') / C-graphite (n,n') elastic scattering and C-graphite (total) / C-graphite (total) nuclide reactions have the three largest sensitivity coefficients. The TSUNAMI integral sensitivity coefficients shown in Table 4-9 are obtained by integrating the region- and mixture-integrated sensitivity coefficients per-unit lethargy (shown in Figure 4-15 for the VHTRC HP core at 473 K) over the 56-group structure listed in Table 10.1.10 in the SCALE User Manual (Rearden et al. 2018). The sensitivity coefficients per-unit lethargy are obtained using Equation (4-1), with the energy bins  $E_2$  and  $E_1$  obtained from the 56-group structure:

$$sens_{leth} = \frac{sens_{coef}}{\ln\left(\frac{E_2}{E_1}\right)} \quad (4-1)$$

The basic nature of the nuclide reactions—e.g. the mean number of neutrons emitted per fission ( $^{235}\text{U}[\bar{\nu}]$ ) sensitivity peaks below 1 eV, and the resonance structure of the  $^{238}\text{U}(n,\gamma)$  reaction—can be seen in this plot.

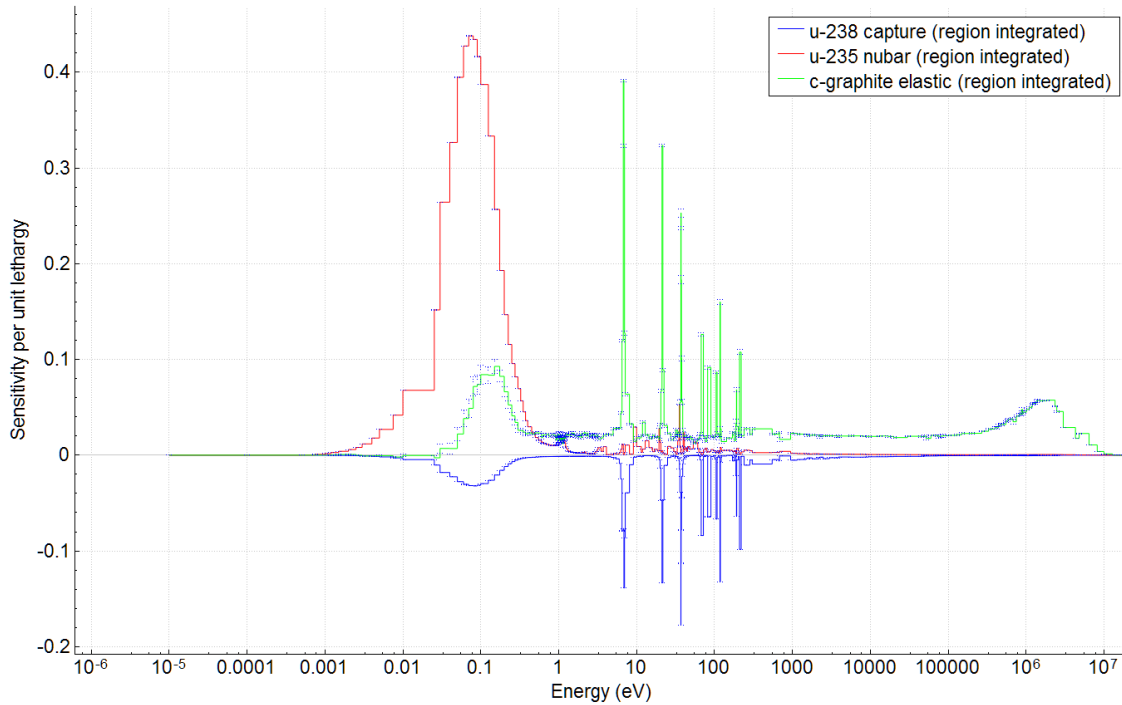


Figure 4-15. TSUNAMI region- and mixture-integrated sensitivity coefficients per-unit lethargy for the VHTRC HP core at 473 K.

In contrast to the perturbation-theory based TSUNAMI sequence, the statistical Sampler module currently does not support sensitivity analysis, and RAVEN is utilised in this research to provide simplified sensitivity indices such as the absolute and normalised sensitivity coefficients (NSCs), covariances and Pearson correlation coefficients (PCCs)<sup>19</sup> for the NEWT/PHISICS/Sampler sequence.

In the Sampler module, the SCALE MG covariance data are given as a set of multiplicative perturbation factors,  $Q_{x,g}$ , as described in Section 3.2.2 and Equation (3-3). The XSUSA data set in Sampler is currently limited to 1,000  $Q_{x,g}$  factors and can be using the SCALE utility routine PaleAle on both the 56- and 252-group covariance libraries. RAVEN can thereby access the perturbed vector of all  $Q_{x,g}$  factors for each of the 1,000 entries in the Sampler data base by combining the eigenvalues for each of the VHTRC cases with the perturbed data for each nuclide reaction of interest.

<sup>19</sup> See Appendix B-1 for definitions of the NSC and PCC sensitivity indices.

The RAVEN NSCs is defined as least-square linear fit coefficients that are normalized with respect to their mean values (see Section B-1 for more detail). Because the mean values of all the group-dependent Sampler  $Q_{x,g}$  factors are equal to 1.0 (see the discussion in B-4), a NSC value of 0.5 for the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction, for example, implies that a perturbation of +1% in the  $Q_{x,g}$  factor will lead to a change of  $0.5 \times 1\% = 0.5\%$  in the eigenvalue<sup>20</sup>.

Table 4-9. VHTRC CE TSUNAMI and NEWT/Sampler/RAVEN eigenvalue-sensitivity coefficients.

| Ranking                                               | Reaction                                                            | HC-1_281 | HP_298 | HP_344 | HP_374 | HP_423 | HP_473 |
|-------------------------------------------------------|---------------------------------------------------------------------|----------|--------|--------|--------|--------|--------|
| CE TSUNAMI integral sensitivity coefficient           |                                                                     |          |        |        |        |        |        |
| 1                                                     | $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$             | 0.993    | 0.993  | 0.993  | 0.993  | 0.993  | 0.993  |
| 2                                                     | C-graphite (n,n') /<br>C-graphite (n,n')                            | 0.609    | 0.574  | 0.615  | 0.603  | 0.581  | 0.589  |
| 3                                                     | C-graphite total / C-graphite total                                 | 0.518    | 0.486  | 0.527  | 0.517  | 0.495  | 0.499  |
| 4                                                     | $^{235}\text{U}(\text{n,f}) / ^{235}\text{U}(\text{n,f})$           | 0.376    | 0.381  | 0.386  | 0.392  | 0.397  | 0.376  |
| 5                                                     | $^{238}\text{U}(\text{n},\gamma) / ^{238}\text{U}(\text{n},\gamma)$ | -0.132   | -0.134 | -0.134 | -0.135 | -0.135 | -0.134 |
| NEWT/Sampler/RAVEN normalised sensitivity coefficient |                                                                     |          |        |        |        |        |        |
| 1                                                     | $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$             | 0.929    | 0.938  | 0.936  | 0.936  | 0.936  | 0.935  |
| 2                                                     | $^{238}\text{U}(\text{n},\gamma) / ^{238}\text{U}(\text{n},\gamma)$ | -0.097   | -0.098 | -0.098 | -0.098 | -0.098 | -0.099 |
| 3                                                     | C-graphite (n,n') /<br>C-graphite (n,n')                            | 0.047    | 0.045  | 0.045  | 0.045  | 0.045  | 0.045  |

It is important to note that because the RAVEN sensitivity indices are basically linear fit correlation coefficients, the individual cross-section uncertainty contributions to the total uncertainty in the eigenvalue cannot be calculated from this data. In TSUNAMI the top contributors are identified by collapsing the sensitivity coefficients with the covariance data, but in the statistical formulation this would require a significant number of additional samples to be performed.

<sup>20</sup> The 1% perturbation is simply chosen as a “unit” perturbation for comparison purposes. In reality, the XSUSA-derived  $Q_{x,g}$  factors vary in accordance with the ENDF covariance data, as for example shown in Figure 3-7. It can be seen here that the standard deviation for the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  is ~100 times smaller than the deviation in  $^{239}\text{Pu}(\text{n},\gamma) / ^{239}\text{Pu}(\text{n},\gamma)$ . A 1% perturbation in  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  is therefore almost 2.5 standard deviations of the  $Q_{x,g}$ , compared to 1/40<sup>th</sup> of the  $^{239}\text{Pu}(\text{n},\gamma) / ^{239}\text{Pu}(\text{n},\gamma)$   $Q_{x,g}$  standard deviation.

Bostelmann (2020) provides an in-depth comparison of three sensitivity methods in her U/SA of SFR systems, and concluded that the correlation-based sensitivity indices (e.g.  $R^2$  or  $SPC^2$ ) provided very similar results with much less effort required to calculate variance-based indices such as Sobol's main sensitivity index (Sobol, 2001). Such a development is beyond the scope of this dissertation, because the primary objective of the present work is to provide an example of the statistical U/SA methodology applied to a prismatic HTGR system, rather than a full sensitivity assessment. The current RAVEN correlation-based sensitivity indices will still allow the identification of the most important input uncertainties and perform a ranking comparison across the various phases and exercise, which could inform future areas of research into uncertainty reduction.

Because the various cross-section reactions sensitivity coefficients are group dependent, 56 RAVEN NSC values are obtained for the SCALE 56-group covariance library. In visual form, the plots shown in Figure 4-16 and Figure 4-17 can be obtained, where the variations in the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  and  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  NSCs for the three core loadings are presented as a function of the group index (1 = fast, 56 = thermal, with the thermal scattering cut-off at 5eV at group 40). Both distributions reach their maximum values in the epithermal energy region, with the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  NSC equal to 0.94 and the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  minimum equal to -0.10 around group 47.

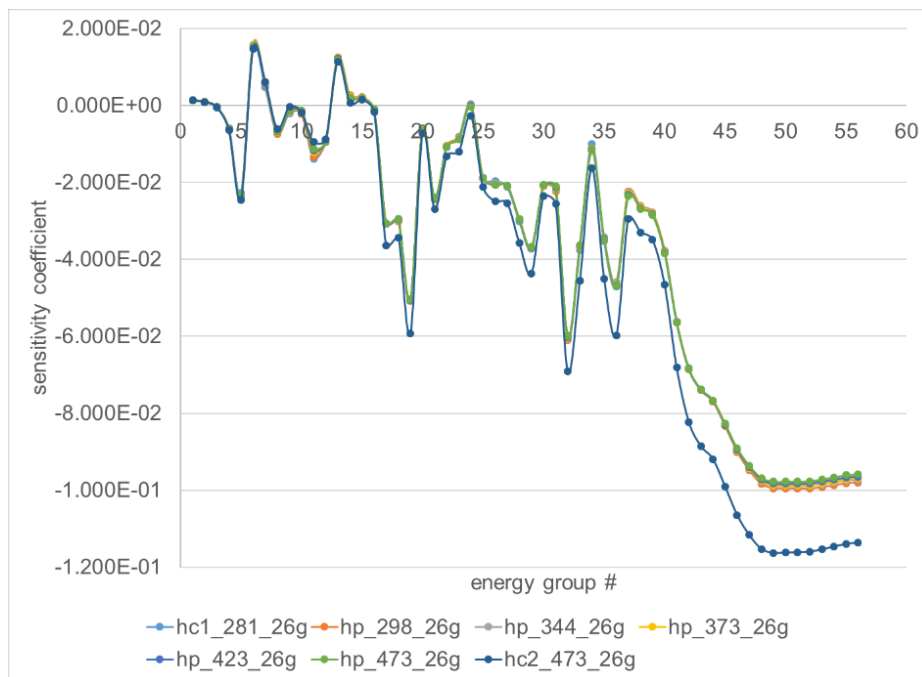


Figure 4-16. Comparison of the RAVEN 56-group  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  NSCs for the VHTRC HC-1, HP, and HC-2 cores.

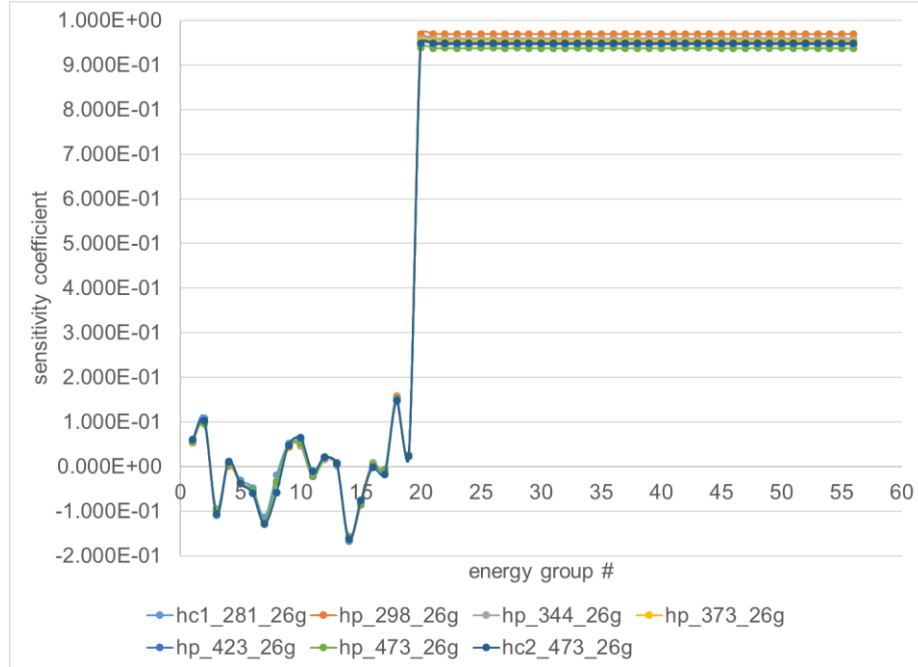


Figure 4-17. Comparison of the RAVEN 56-group  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  NSCs for the VHTRC HC-1, HP, and HC-2 cores.

The TSUNAMI integral sensitivity coefficients cannot be compared with the least-square linear fit sensitivity coefficients determined by RAVEN, because TSUNAMI utilizes a global adjoint GPT approach to determine the sensitivity contributions, whereas RAVEN lacks a global variance decomposition method like Sobol's (Sobol, 2001) to calculate a comparative sensitivity metric. The absolute values of the two data sets in Table 4-9 should therefore not be compared, but a comparison of the relative rankings of these sensitivity coefficients can nevertheless be performed.

It can be seen in Table 4-9 that although the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction is ranked first for both TSUNAMI and Sampler/RAVEN, the relative ranking of the RAVEN  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  integral NSC is higher than the C-graphite (n, n') / C-graphite (n, n') NSC, while the TSUNAMI order of these two reactions is reversed. The RAVEN coefficients are however both small and the difference between these two sensitivities are probably not significant, especially if the limitations of the RAVEN method is kept in mind (the NEWT/Sampler sequence uses a much-coarser energy structure (26-groups) than TSUNAMI and also only has indirect access to the covariances through the 1,000 perturbed  $Q_{x,g}$  factors).

Finally, a determination can also be made on the relative contributions of each nuclide reaction to total uncertainty in the VHTRC PHYSICS eigenvalue. At this stage, this capability is not available in RAVEN, but TSUNAMI results are shown for the VHTRC cores in Table 4-10.

The top three nuclide reactions that contribute to the eigenvalue uncertainty are the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ , C-graphite (n,n') and C-graphite (n, $\gamma$ ) reactions, with the graphite contributions expected due to the large carbon-to-fuel ratios in the VHTRC and the uncertainties of the C-graphite elastic scatter and capture cross-sections. For the ENDF/B.VII library, the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  covariance was increased in the thermal energy range from 0.311% to 0.385%. Since the eigenvalue is very sensitive to  $^{235}\text{U}(\bar{\nu})$  as the primary neutron source term in the transport equation, the update of this covariance value has a significant impact on the eigenvalue uncertainty.

Table 4-10. CE TSUNAMI top five contributions to the eigenvalue uncertainty by individual covariance matrices.

| Covariance matrix                                       | Contribution to eigenvalue uncertainty (% $\Delta k/k$ ) |        |        |        |        |        |
|---------------------------------------------------------|----------------------------------------------------------|--------|--------|--------|--------|--------|
|                                                         | HC-1                                                     | HP_298 | HP_344 | HP_374 | HP_423 | HP_473 |
| $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ | 0.379                                                    | 0.379  | 0.379  | 0.379  | 0.379  | 0.379  |
| C-graphite (n,n') / C-graphite (n,n')                   | 0.303                                                    | 0.285  | 0.306  | 0.300  | 0.289  | 0.293  |
| C-graphite (n, $\gamma$ ) / C-graphite (n, $\gamma$ )   | 0.279                                                    | 0.272  | 0.269  | 0.264  | 0.269  | 0.276  |
| $^{235}\text{U} \chi / ^{235}\text{U} \chi$             | 0.192                                                    | 0.190  | 0.190  | 0.189  | 0.188  | 0.191  |
| $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$   | 0.181                                                    | 0.184  | 0.184  | 0.184  | 0.185  | 0.184  |

## 4.5 Conclusion

The application of the code sequence Sampler/NEWT/PHISICS to the simulation of the VHTRC experiment demonstrated the viability of using this statistical-perturbation method for the uncertainty and sensitivity assessment of HTGR systems. This U/SA sequence will be applied in Chapters 5–8 on the MHTGR-350 design, and this chapter on the VHTRC is intended to at least partially validate the methodology as being capable of capturing the important aspects of the experimental data set. The scope of the U/SA was limited to the evaluation of cross-section uncertainties on the eigenvalues of three VHTRC-core loadings and at six temperature points. Although the VHTRC is a low-enriched, low-temperature system with a high graphite-to-fuel ratio, the experimental data set is valuable for the inclusion of uncertainty estimates by the IRPhEP benchmark evaluators.

For the VHTRC uncertainty assessment, a sample consisting of 1,000 NEWT/PHISICS calculations was created for each core variant using the XSUSA-generated perturbation factors in the Sampler module of SCALE 6.2. The 252-group ENDF/B-VII.1 library was used to create 26- and 8-group collapsed libraries for use in the PHISICS models, and statistical analysis was performed with the RAVEN code.

It was found that the 26-group results matched the experimental data significantly better than the 8-group data, but for the assessment of cross-section uncertainties, the 8-group structure produces identical eigenvalue uncertainties to the 26-group models (0.63%). The use of the 8-group structure in Chapter 8 for the U/SA of the MHTGR-350 transients is therefore justified if best-estimate nominal values are not the focus.

A comparison against independent KENO-VI 252-group models showed that the 252g KENO-VI data agrees better with the experimental data (0.36–0.58% difference) than the 26g PHISICS data (0.46–0.97%), which is seen as quite acceptable for a deterministic 26-group solution. The relative difference between the calculated PHISICS and experimental mean eigenvalues ranged from -0.46 to 0.97%, and for most cases the PHISICS simulations agree with the experimental data within  $2\sigma$  of the experimental uncertainty. The main observation was that regardless of the VHTRC-core loading and temperature, the uncertainties in the cross-sections led to an uncertainty of 0.64% in the PHISICS eigenvalue. This result is very well matched with the Sampler/KENO-VI and TSUNAMI model predictions of 0.66%. Because the NEWT and KENO-VI models were independently developed, and both statistical (Sampler) and deterministic (TSUNAMI) methods were used, this provides a very good verification basis for the use of the Sampler/NEWT/PHISICS sequence.

A comparison with work performed by Rouxelin (2019) on the impact of manufacturing uncertainties led to the conclusion that the cross-section uncertainties lead to larger uncertainties in the VHTRC eigenvalues (631–654 pcm) than manufacturing uncertainties (233–346 pcm). The contributions of each of these input uncertainties to the total calculation uncertainty can only be assessed, however, by combining all known input uncertainties in a consistent and simultaneous statistical-uncertainty assessment, which was beyond the scope of the current work.

In terms of the sensitivity analysis, roughly similar trends were observed compared to the deterministic TSUNAMI results, but the sensitivity coefficients cannot be compared between the TSUNAMI and RAVEN approaches. (A variance decomposition method like Sobol's (2001) would need to be applied to the RAVEN data before a direct comparison of the sensitivity data is performed). It was shown that the primary sensitivity coefficient was the same for both approaches ( $^{235}\text{U}[\bar{\nu}] / ^{235}\text{U}[\bar{\nu}]$ ), but the relative ranking of the next two largest integral sensitivity coefficients ( $^{238}\text{U}[n,\gamma] / ^{238}\text{U}[n,\gamma]$  and C-graphite  $[n,n'] / \text{C-graphite } [n,n']$ ) were reversed. The top three nuclide reactions that contribute to the eigenvalue uncertainty were identified in the TSUNAMI analysis as the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ , C-graphite  $(n,n') / \text{C-graphite } (n,n')$  and C-graphite  $(n,\gamma) / \text{C-graphite } (n,\gamma)$  reactions.

## 5. MHTGR-350 EXERCISE I-1: LATTICE NEUTRONICS

*"An approximate answer to the right problem is worth a good deal more than an exact answer to an approximate problem." John Tukey.*

The use of unit cells arranged in a lattice configuration for the generation of few-group cross-sections that can be used in steady-state and transient core analysis is standard practice in reactor physics. For LWRs, a lattice calculation can be based on the same geometry as the standard LWR fuel assembly because the moderation ratio of water is sufficiently high that high-energy (fast) neutrons generated inside the fueled region are thermalized within one or two interactions with hydrogen. As indicated in Section 2.2.2, the situation is different in HTGRs, where the moderation ratio of graphite leads to longer neutron migration lengths (Table 2-2), and the definition of lattice cells for cross-section generation is more complex.

The focus of this chapter is on the generation of suitable lattice models that can be used to construct the perturbed P/R core models, utilizing the NEWT/Sampler statistical U/SA sequence described in Section 3.2.2. RAVEN is only used in this chapter to determine sensitivity indices, and the ranking of the main cross-section uncertainty contributors will be compared with TSUNAMI values because statistical-sensitivity indices based on the Sampler sequence are not yet available in SCALE. The statistical U/SA results are compared for the lattice cases with the deterministic U/SA data obtained with TSUNAMI in terms of mean and standard-deviation eigenvalue uncertainties.

A summary of the applicable IAEA CRP on HTGR UAM specifications for Phase I is provided in Section 5.1. This is followed in Section 5.2.1 by a short overview of the nominal Serpent2, KENO-VI, NEWT results obtained for the single block (Ex. I-2a and Ex. I-2b) and supercell (Ex. I-2c) lattice models, with the aim of introducing the reference models used for the NEWT/Sampler/RAVEN statistical U/SA sequence. The NEWT/Sampler and TSUNAMI U/SA results for the neutronics stand-alone lattice models are reported in Section 5.2.2.

### 5.1 Specification of the IAEA CRP on HTGR UAM Stand-Alone Neutronics Cases

The IAEA CRP on HTGR UAMs benchmark consists of specifications for both pebble-bed and prismatic HTGR core designs. The prismatic specifications were developed by the author as principle investigator for the U.S., with support provided by Friederike Bostelmann (ORNL) and Pascal Rouxelin (NCSU) in the period 2014–2018 (see Appendix C for more detail). Development of a benchmark specification development is seen as one of the major contributions of the Ph.D. research reported in this dissertation. The three subsections below provide a condensed summary based on the detailed IAEA CRP on HTGR UAM specifications (Strydom et al. 2015).

### 5.1.1 Phase I Exercises I-2a & I-2b: Lattice Neutronics (Fresh and Depleted Single Blocks)

The geometry and isotopic data for the simplified single MHTGR-350 hexagonal fuel block (Figure 5-1) are specified in Table 5-1 and Table 5-2. The fresh fuel block defined for Exercise I-2a includes six LBP compacts in the six corners of the block. For the depleted fuel block defined for Exercise I-2b it is assumed that all LBPs have been fully depleted and are replaced by H-451 block graphite. Both exercises require treatment of the double-heterogeneity effects, i.e. the self-shielding that occurs both within the fuel and LBP compacts, as well as the effect of multiple compacts present in a single block.

The full set of 279 nuclide densities for the depleted fuel kernels is provided in the benchmark specifications. The nuclide densities were obtained by performing a Serpent2 depletion calculation of the Exercise I-2a fresh block without LBPs up to 100 MWd/kg-U (see Strydom and Bostelmann, 2017 for more detail). Only HFP conditions at 1,200 K are considered for these two exercises.

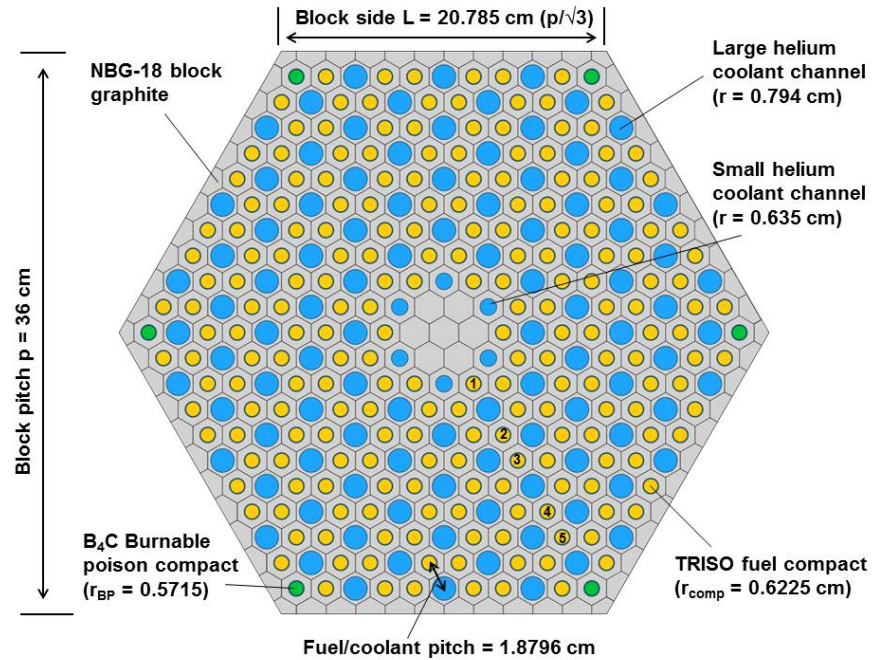


Figure 5-1. MHTGR-350 fuel block (and lattice cell for Exercise I-2).

Table 5-1. TRISO and block dimensions for Exercise I-2.

| Parameter                         |                                                  | Dimension | Units |
|-----------------------------------|--------------------------------------------------|-----------|-------|
| TRISO fuel particle               | UC <sub>0.5</sub> O <sub>1.5</sub> kernel radius | 2.125E-02 | cm    |
|                                   | Porous carbon buffer outer radius                | 3.125E-02 | cm    |
|                                   | IPyC OR                                          | 3.525E-02 | cm    |
|                                   | SiC OR                                           | 3.875E-02 | cm    |
|                                   | OPyC OR                                          | 4.275E-02 | cm    |
| TRISO packing fraction            |                                                  | 0.35      | —     |
| Fuel-compact radius               |                                                  | 6.225E-01 | cm    |
| Gap radius                        |                                                  | 6.350E-01 | cm    |
| Number of fuel compacts per block |                                                  | 210       | —     |
| LBP particle                      | Kernel radius                                    | 1.000E-02 | cm    |
|                                   | Porous carbon buffer outer radius                | 1.180E-02 | cm    |
|                                   | PyC outer radius                                 | 1.410E-02 | cm    |
| BP particle packing fraction      |                                                  | 0.11      |       |
| BP compact radius                 |                                                  | 5.715E-01 | cm    |
| Large coolant channel radius      |                                                  | 7.940E-01 | cm    |
| Number of large coolant holes     |                                                  | 102       | —     |
| Small coolant channel radius      |                                                  | 6.350E-01 | cm    |
| Number of small coolant holes     |                                                  | 6         | —     |
| Pin pitch                         |                                                  | 1.88      | cm    |
| Block flat-to-flat width          |                                                  | 36.00     | cm    |
| Block (compact) height            |                                                  | 4.93      | cm    |

### 5.1.2 Phase I Exercise I-2c: Lattice Neutronics (Supercell)

The use of reflective boundary conditions for single fuel blocks next to the inner or outer reflectors leads to significant spectral variances because these blocks are not surrounded by an infinite lattice of fuel blocks (Descotes et al. 2012). To investigate the effect of neighbouring blocks on the uncertainties impacting a typical lattice calculation, an example of a supercell or minicore has been defined as presented in Figure 5-2.

In this example, Block 26 is surrounded by reflector blocks on the right and top boundaries, and by one fresh and two depleted<sup>21</sup> fuel blocks on the left and lower boundaries. The non-central fuel blocks are homogenized using the relative contributions of two depleted fuel blocks and one fresh fuel block, as shown on the right of Figure 5-2. Only the central fresh fuel block is required to be modeled in heterogeneous detail (LBP and TRISO compacts), using the geometry and number-density data provided for Exercises I-2a and I-2b. Rouxelin (2019) showed that the use of homogenized neighbouring blocks to represent the spectral environment of the central block has an insignificant impact on central block cross-sections.

A trace amount of neutron-absorber impurities has been added to the reflector graphite and represented as homogenized <sup>10</sup>B-equivalent boron content. It is assumed that these impurities do not deplete over time. In order to reduce the amount of required calculation memory, the supercell calculation is specified using 94 nuclides instead of the full Serpent2 list of 285 nuclides. This reduced set of 94 depleted number densities is provided in the benchmark specifications.

Table 5-2. Nuclide densities for the fresh (Exercise I-2a) and depleted (Exercise I-2b) fuel blocks.

| Nuclide Densities             |                                                           | Nuclide                                          | N (at/b-cm)                                      |
|-------------------------------|-----------------------------------------------------------|--------------------------------------------------|--------------------------------------------------|
| TRISO fuel particle           | UC <sub>0.5</sub> O <sub>1.5</sub> kernel (fresh fuel)    | <sup>235</sup> U                                 | 3.6676E-03                                       |
|                               |                                                           | <sup>238</sup> U                                 | 1.9742E-02                                       |
|                               |                                                           | <sup>16</sup> O                                  | 3.5114E-02                                       |
|                               |                                                           | Graphite                                         | 1.1705E-02                                       |
|                               | UC <sub>0.5</sub> O <sub>1.5</sub> kernel (depleted fuel) | See specifications (Strydom and Bostelmann 2017) | See specifications (Strydom and Bostelmann 2017) |
|                               | Porous carbon                                             | Graphite                                         | 5.2646E-02                                       |
|                               | IPyC                                                      | Graphite                                         | 9.5263E-02                                       |
|                               | SiC                                                       | <sup>28</sup> Si                                 | 4.4159E-02                                       |
|                               |                                                           | <sup>29</sup> Si                                 | 2.2433E-03                                       |
|                               |                                                           | <sup>30</sup> Si                                 | 1.4805E-03                                       |
|                               |                                                           | Graphite                                         | 4.7883E-02                                       |
|                               | OPyC                                                      | Graphite                                         | 9.5263E-02                                       |
| BP particle (fresh fuel only) | Kernel                                                    | <sup>10</sup> B                                  | 2.1400E-02                                       |
|                               |                                                           | <sup>11</sup> B                                  | 8.6300E-02                                       |

<sup>21</sup> “Burned” and “depleted” are both used in MHTGR-350 benchmark publications.

| Nuclide Densities    |        | Nuclide         | N (at/b-cm) |
|----------------------|--------|-----------------|-------------|
|                      |        | Graphite        | 2.6900E-02  |
|                      | Buffer | Graphite        | 5.0200E-02  |
|                      | PyC    | Graphite        | 9.3800E-02  |
| Fuel compact matrix  |        | Graphite        | 7.2701E-02  |
| LBP compact matrix   |        | Graphite        | 7.2701E-02  |
| Coolant channels     |        | $^4\text{He}$   | 2.4600E-05  |
| H-451 block graphite |        | Graphite        | 9.2756E-02  |
|                      |        | $^{10}\text{B}$ | 2.7600E-08  |

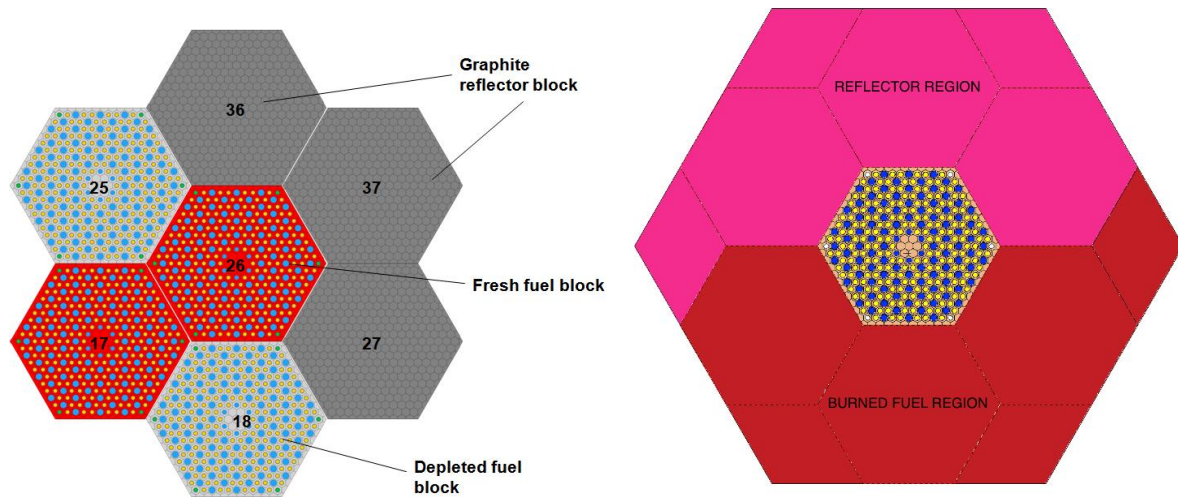


Figure 5-2. MHTGR-350 supercell centered at Block 26 (left) and simplified representation (right).

## 5.2 Phase I Exercise I-2: Lattice Neutronics Results

The U/SA of the MHTGR-350 lattice exercises, as defined in the Phase I specifications (Strydom et al. 2015), starts with the generation of nominal<sup>22</sup> KENO-VI, NEWT and Serpent2 models and results. The same models are subsequently used in the deterministic TSUNAMI (KENO-VI) and statistical Sampler (KENO-VI and NEWT) sequences to assess the overall uncertainties and identify the main sensitivity drivers. In the context of this work, and in the absence of experimental data, the Serpent2 nominal results using random distributions of TRISO fuel particles are used as the basis for comparison against the KENO-VI and NEWT nominal results.

<sup>22</sup> All input parameters are set at nominal, or best-estimate, values.

### 5.2.1 Nominal Results

The discussion of the nominal results in this section is intended to highlight the fact that other sources of uncertainty exists apart from uncertainties in nuclear data, boundary conditions or thermal fluid parameters. An important source of uncertainty or bias is the user's choice of reactor simulation code for a specific reactor and application (e.g. Monte Carlo vs deterministic transport, or even the choice between two Monte Carlo codes). Once a reactor physics code has been selected, various model approaches, energy group representations and heterogeneity treatments can be implemented. One example available in some Monte Carlo codes such as Serpent2 and MCNP is the choice to represent the TRISO fuel particles using a stochastic random distribution (closest to reality), or as a regular lattice array (an obvious approximation). These code and model choices are fully deterministic (i.e. not statistical) and can therefore not be combined with the other statistical uncertainty sources within the static propagation methodology followed in this work. It is however instructive to compare the impact of these code and model choices with the uncertainties calculated in Section 5.2.2 to obtain a more complete picture of the total uncertainties inherent in the HTGR simulation chain.

#### ***Single-block and supercell models***

The Serpent2 fresh-fuel-block model for Exercise I-2a consists of a lattice of unit cells for each of the components (fuel compact, helium-coolant channel, BP, and graphite), and simulations with both random and regular TRISO and BP particle distributions were performed. Reflective boundary conditions were applied in all directions. For each simulation, 500 active neutron cycles with 500,000 neutrons per cycle were calculated. The first 50 cycles were skipped and not considered in the evaluation of the multiplication factor.

The KENO-VI model for Exercise I-2a is similar to the regular lattice Serpent2 model. The reflective boundary condition was retained, and for the MG calculations, the “Doublehet” cell data were specified to consider the double heterogeneous structure of the TRISO particles in the fuel compact. The BP particles were explicitly modeled in a lattice in both the CE and MG calculation because a “Doublehet” treatment is currently not possible for nonfueled particles in SCALE. The self-shielding effects of the BP particles were thus neglected in the MG model. For each simulation, 500 active neutron cycles with 50,000 neutrons per cycle were calculated and 50 cycles were skipped.

The Serpent2 and KENO-VI models were both developed by Friederike Bostelmann in 2015, and the nominal results obtained with earlier versions of SCALE were reported in Bostelmann, Strydom, and Yoon 2015, and Bostelmann et al. 2016a. The NEWT models for Phase I were created by Rouxelin as part of his Ph.D. research (Rouxelin 2019).

Since NEWT is only capable of 2D simulation, the BP particles cannot be modeled explicitly, as is the case in KENO-VI, requiring, instead, a homogenization of the  $B_4C$  particles over the volume of the BP compact. Although this approximation introduces significant errors in the local reactions rates and the overall eigenvalue due to the neglect of particle self-shielding in the BP compact, the effect on the neutron spectrum and the few-group cross-sections generated for Phase II is limited (Rouxelin and Strydom 2017). The NEWT models of the fresh fuel block (Ex. I-2a) and the supercell (Ex. I-2c) are shown in Figure 5-3 (left). The Serpent2, KENO-VI, and NEWT models of Ex. I-2a and I-2b are identical, with only the fuel compositions replaced by the respective depleted compositions and without the BP compacts. Details on the assumptions made for the Serpent2 burnup calculation can be found in the Phase I specifications.

For the supercell calculation, the depleted number densities for the homogenized burned fuel blocks were obtained from the Serpent2 burnup calculation performed in Exercise I-2b. The Ex. I-2c NEWT supercell model consists of a lattice of one fresh fuel block (Ex. I-2a), the homogenized depleted fuel blocks, and graphite reflector blocks, as shown in Figure 5-3 (right). The depleted region consists of a homogenous mixture of two depleted and one fresh fuel blocks. Reflective boundary conditions were applied, and the simulations used 500,000 neutrons in 500 active and 50 skipped cycles. For KENO-VI, the same settings as Ex. I-2a/2b were used.

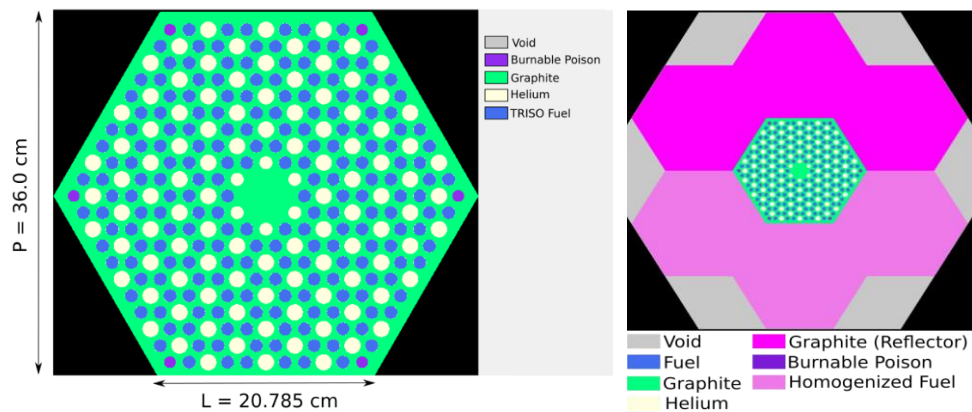


Figure 5-3. NEWT 2D representation of the Ex. I-2a fresh fuel block (left) and Ex. I-2c supercell (right) (Rouxelin 2019).

**Phase I nominal results**

The nominal multiplication factors obtained for the Serpent2, KENO-VI, and NEWT models of Ex. I-2a, I-2b and I-2c are summarized in Table 5-3. All models used the ENDF/B-VII.1 library available in the SCALE 6.2.0 release, and the Serpent2 calculation with a random particle distribution is used as the reference<sup>23</sup> result.

The impact of a regular lattice approach can clearly be seen if the CE KENO-VI results are compared with the two different Serpent2 results. The three KENO-VI CE models overestimate the respective Serpent2 random-model eigenvalues by 0.42–0.56%, but the agreement with the Serpent2 lattice model is significantly better (0.09–0.38%). The differences between the random and lattice Serpent2 eigenvalues can be attributed to the change in the average distance between the fuel particles and the resultant decrease in spatial self-shielding. In terms of the context of the current study on HTGR UAM, these differences fall in the category of model/method uncertainties. These uncertainties are not statistical (e.g. the decision of the user to select one code or method instead of another) and are not treated as part of the statistical propagation methodology. These modeling uncertainties are considered as biases that the user needs to be aware of, e.g. in this case the use of a KENO-VI lattice model has been shown to produce a ~0.5% bias/trend compared with a random Serpent2 model.

A comparison of the normalized flux-spectrum per-unit lethargy for the heterogeneous unit cell (Ex. I-1b), the single blocks (I-2a, I-2b) and the supercell (I-2c) is presented in Figure 5-4 (Bostelmann, Strydom, and Yoon 2015). The unit cell exhibits the hardest spectrum due to the lowest moderator-to-fuel ratio (as defined in the benchmark, the unit cell does not contain the correct block-averaged moderator-to-fuel ratio), but the spectrum for the fresh fuel block is also relatively hard due to the increased absorption of thermal neutrons by in the BP compacts.

In contrast to the fresh fuel block, the Ex. I-2b depleted fuel block has a much-larger thermal peak, primarily caused by the depletion of  $^{238}\text{U}$  in Ex. I-2b and the subsequent reduced  $^{238}\text{U}$  resonance absorption. In addition, the removal of the  $\text{B}_4\text{C}$  absorber compacts from the depleted block also increased the thermal neutron population. Figure 5-4 also shows the difference between the total radiative capture ( $n,\gamma$ ) macroscopic cross-section in the depleted and fresh fuel blocks, where the effect of the  $^{239}\text{Pu}$  ( $n,\gamma$ ) cross-section (Figure 5-5) can clearly be seen at ~0.5 eV. The sharp decrease in the capture cross-section at ~50 eV is likewise caused by the depletion of  $^{238}\text{U}$  in Ex. I-2b and the subsequently reduced  $^{238}\text{U}$  resonance absorption.

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<sup>23</sup> Serpent is used as a reference in the sense that it is the basis for relative comparison, not the “best”.

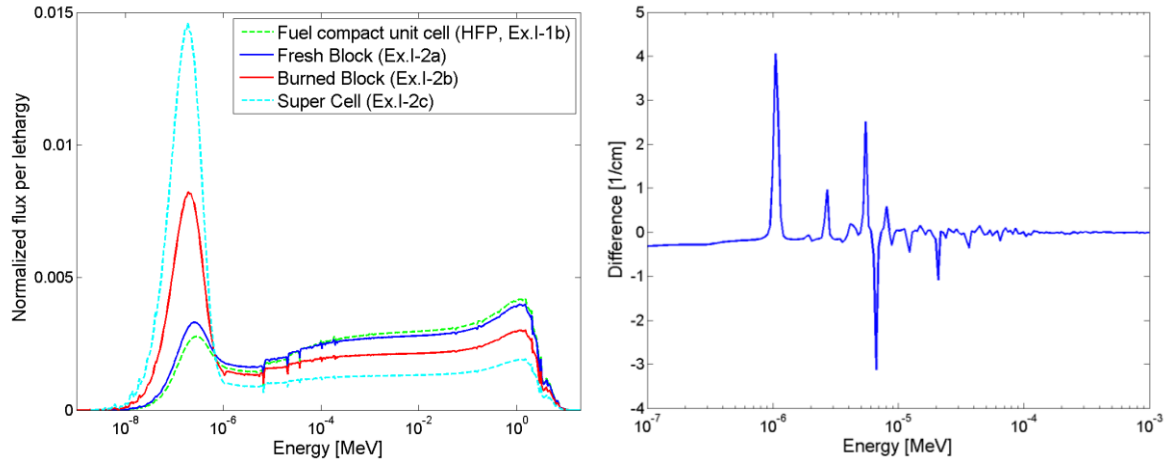


Figure 5-4. Normalized neutron-flux per-unit lethargy for the MHTGR-350 unit cell, single block, and supercell lattices (left), and difference between the total macroscopic capture ( $n,\gamma$ ) cross-section of the burned and fresh fuel block (right) (Bostelmann, Strydom, and Yoon 2015).

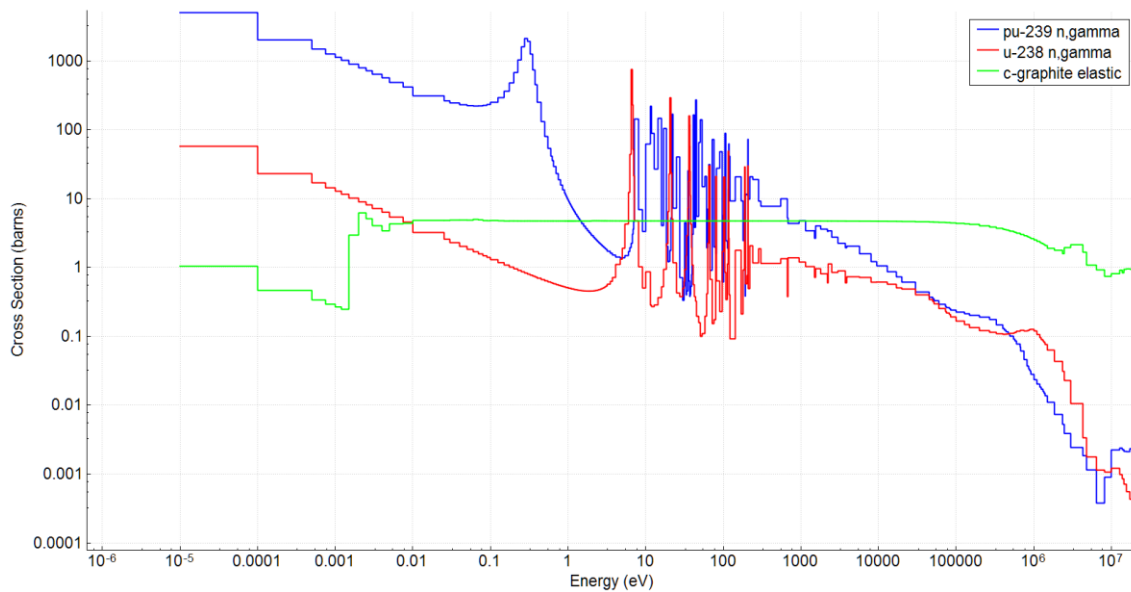


Figure 5-5. ENDF/B VII.1 cross-sections for  $^{239}\text{Pu}$  ( $n,\gamma$ ),  $^{238}\text{U}$  ( $n,\gamma$ ) and C-graphite ( $n,n'$ ).

The effect of the homogenization of the LBP compacts was also quantified by performing an additional KENO-VI 252 MG calculation (5<sup>th</sup> row of Table 5-3). The homogenization of the LBPs into the rest of the fuel-block lattice led to a significant decrease in  $k_\infty$  ( $\sim 1.4\%$ ) compared to the heterogenous BP KENO-VI result, caused by the neglect of the spatial self-shielding effects. The NEWT model uses the same approximation, and it can be seen in Table 5-3 that most of NEWT's underestimation ( $-0.48\%$ ) can be attributed to the BP homogenization effect by comparing the relative results of Ex. I-2a (BPs included) and I-2b/I-2c (no BPs).

Table 5-3. Nominal  $k_{\infty}$  data for Exercises I-2a, I-2b and I-2c.

| Model                          |         | $\sigma$ | $\Delta k$ (pcm) <sup>24</sup> | % $\Delta k/k$ |
|--------------------------------|---------|----------|--------------------------------|----------------|
| I-2a                           |         |          |                                |                |
| Serpent2 – random              | 1.05559 | 0.00025  | reference                      | reference      |
| Serpent2 – lattice             | 1.05997 | 0.00024  | 438                            | 0.415          |
| KENO-VI CE                     | 1.06140 | 0.00019  | 581                            | 0.550          |
| KENO-VI 252 MG                 | 1.05995 | 0.00013  | 436                            | 0.413          |
| KENO-VI 252 MG homogenized BPs | 1.04699 | 0.00011  | -860                           | -0.815         |
| NEWT 252 MG                    | 1.05059 | -        | -500                           | -0.474         |
| I-2b                           |         |          |                                |                |
| Serpent2 – random              | 0.96126 | 0.00018  | reference                      | reference      |
| Serpent2 – lattice             | 0.96617 | 0.00018  | 491                            | 0.511          |
| KENO-VI CE                     | 0.96534 | 0.00019  | 408                            | 0.424          |
| KENO-VI 252 MG                 | 0.96393 | 0.00012  | 267                            | 0.278          |
| NEWT 252 MG                    | 0.96314 | -        | 188                            | 0.196          |
| I-2c                           |         |          |                                |                |
| Serpent2 – random              | 1.06283 | 0.00010  | reference                      | reference      |
| Serpent2 – lattice             | 1.06471 | 0.00011  | 188                            | 0.177          |
| KENO-VI CE                     | 1.06874 | 0.00016  | 591                            | 0.556          |
| KENO-VI 252 MG                 | 1.06482 | 0.00013  | 199                            | 0.187          |
| NEWT 252 MG                    | 1.06332 | -        | 49                             | 0.046          |

## 5.2.2 Exercise I-2 Uncertainty and Sensitivity Results

The uncertainty and sensitivity assessment of Phase I lattice models were investigated using both deterministic (CE TSUNAMI) and statistical (MG Sampler) SCALE modules. The CE TSUNAMI models utilized the CLUTCH approach (Rearden et al. 2018) and the 56-group cross-section covariance library to calculate the uncertainty on  $k_{\infty}$ . CLUTCH is based on GPT and calculates sensitivity coefficients during a single forward KENO-VI simulation. Unlike MG TSUNAMI-3D, this approach does not require the simulation of adjoint histories or treatment of implicit sensitivity effects, which occurs when a perturbation in the cross-section of a nuclide changes the self-shielded cross-section of another nuclide (Bostelmann et al. 2016).

The Sampler module of SCALE 6.2 utilizes the multiplicative perturbation factors,  $Q_{x,g}$  generated by the XSUSA code (as described in Section 2.4.2 and Equation 2-13) to produce up to 1,000 perturbed 252-group ENDF/B-VII.1 cross-section libraries for use in the deterministic NEWT or Monte Carlo KENO-VI calculations. Sampler is currently not able to compute sensitivity indices.

<sup>24</sup> 1 pcm = 1 per cent mille. 1 pcm  $\Delta k$  = 0.00001  $\Delta k$ .

Following the calculation sequence shown in Figure 2-15, RAVEN was therefore used as a statistical post-processor to compute various indices of interest, such as the sample mean ( $\mu$ ), standard deviation ( $\sigma$ ), sensitivity coefficients and PCCs for selected cross-section reaction pairs. The mean value is usually expressed in relation to a sample-dependent confidence interval (see Section 3.2.2.2).

### TSUNAMI Results

The TSUNAMI best-estimate  $k_{\infty}$  and standard deviations obtained for Ex. I-2a, I-2b and I-2c are summarized in Table 5-4, along with the nuclide-reaction covariance matrices responsible for the five largest contributions to the  $k_{\infty}$  uncertainties. The  $k_{\infty}$  relative standard deviations due to the cross-section covariance data vary between 0.50–0.54% for these cases, which is similar to the results obtained for Phase I of the OECD LWR UAM benchmark (Mercatali, Ivanov, and Sanchez 2013).

Table 5-4. TSUNAMI  $k_{\infty}$  results for Ex. I-2a and I-2b.

| Rank     | Nuclide-reaction pair                                             | Uncertainty contribution due to this nuclide reaction (% $\Delta k/k$ ) | $k_{\infty} \pm$ statistical standard deviation ( $\sigma_s$ ) (KENO-VI) | $k_{\infty}$ standard deviation due to nuclide-reaction covariance data ( $\sigma_{cov}$ ) (% $\Delta k/k$ ) | total standard deviation ( $\sigma_t$ ) (% $\Delta k/k$ ) |
|----------|-------------------------------------------------------------------|-------------------------------------------------------------------------|--------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------|
| Ex. I-2a |                                                                   |                                                                         |                                                                          |                                                                                                              |                                                           |
| 1        | $^{235}\text{U}(\overline{\nu}) / ^{235}\text{U}(\overline{\nu})$ | 0.357                                                                   | 1.06101 (10)<br><sup>25</sup>                                            | 0.502                                                                                                        | 0.502                                                     |
| 2        | $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$             | 0.198                                                                   |                                                                          |                                                                                                              |                                                           |
| 3        | $^{235}\text{U}(n,\gamma) / ^{235}\text{U}(n,\gamma)$             | 0.178                                                                   |                                                                          |                                                                                                              |                                                           |
| 4        | C-graphite (n,n`) / C-graphite (n,n`)                             | 0.141                                                                   |                                                                          |                                                                                                              |                                                           |
| 5        | $^{235}\text{U} (n,f) / ^{235}\text{U}(n,\gamma)$                 | 0.119                                                                   |                                                                          |                                                                                                              |                                                           |
| Ex. I-2b |                                                                   |                                                                         |                                                                          |                                                                                                              |                                                           |
| 1        | $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$             | 0.197                                                                   | 0.96605 (9)                                                              | 0.544                                                                                                        | 0.544                                                     |
| 2        | C-graphite (n,n`) / C-graphite (n,n`)                             | 0.193                                                                   |                                                                          |                                                                                                              |                                                           |
| 3        | $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$           | 0.189                                                                   |                                                                          |                                                                                                              |                                                           |
| 4        | $^{239}\text{Pu}(n,f) / ^{239}\text{Pu}(n,\gamma)$                | 0.179                                                                   |                                                                          |                                                                                                              |                                                           |
| 5        | $^{239}\text{Pu}(n,f) / ^{239}\text{Pu}(n,f)$                     | 0.151                                                                   |                                                                          |                                                                                                              |                                                           |
| Ex. I-2c |                                                                   |                                                                         |                                                                          |                                                                                                              |                                                           |
| 1        | $^{235}\text{U}(\overline{\nu}) / ^{235}\text{U}(\overline{\nu})$ | 0.255                                                                   | 1.06332 (15)                                                             | 0.510                                                                                                        | 0.510                                                     |
| 2        | C-graphite (n,n`) / C-graphite (n,n`)                             | 0.252                                                                   |                                                                          |                                                                                                              |                                                           |
| 3        | $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$             | 0.193                                                                   |                                                                          |                                                                                                              |                                                           |
| 4        | C-graphite (n, $\gamma$ ) / C-graphite (n, $\gamma$ )             | 0.129                                                                   |                                                                          |                                                                                                              |                                                           |
| 5        | $^{235}\text{U}(n,\gamma) / ^{235}\text{U}(n,\gamma)$             | 0.123                                                                   |                                                                          |                                                                                                              |                                                           |

<sup>25</sup> Compact notation used: 1.06101 (10) = 1.06101  $\pm$  0.00010

The total  $k_{\infty}$  standard deviation  $\sigma_t$  can be obtained by adding the statistical uncertainty  $\sigma_s$  obtained from the forward KENO-VI result to the uncertainty contributions from the covariance data ( $\sigma_{cov}$ ) using the root of sum of squares method. In the case of Ex. I-2a, for example, the total  $k_{\infty}$  standard deviation is  $\sqrt{0.096^2 + 0.5023^2} = 0.5023$ . In practice, if the Monte Carlo calculation is performed using a sufficiently large neutron population, the statistical-sampling uncertainty can be reduced to less than 10 pcm, and the total  $k_{\infty}$  standard deviation is dominated by the  $\sigma_{cov}$  contribution.

In terms of the nuclide covariance-matrix contributors to the uncertainty in  $k_{\infty}$ , the largest Ex. I-2a contributor is the covariance for the  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$  reaction, followed by the  $^{238}\text{U}(n,\gamma)/^{238}\text{U}(n,\gamma)$  (radiative capture) reaction. Here,  $\bar{\nu}$  is the average number of neutrons released per fission. The Ex. I-2b depleted fuel block  $k_{\infty}$  uncertainty contributors also include the capture and fission reactions from the resonance absorber  $^{239}\text{Pu}$  (the fresh block does not contain any  $^{239}\text{Pu}$ ), and for all three lattice cells the C-graphite elastic-scatter reactions contribute significantly to the uncertainty in  $k_{\infty}$ . The differences between the HTGR and LWR/BWR Phase I results are mainly observed in the relative importance of the C-graphite and  $^{238}\text{U}$  elastic scattering contributions, as can be expected from a graphite-moderated thermal system (Bostelmann et al. 2016).

The sensitivity coefficient profiles for the  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$ ,  $^{238}\text{U}(n,\gamma)$ ,  $^{239}\text{Pu}(n,\gamma)/^{239}\text{Pu}(n,\gamma)$  and C-graphite elastic-scatter reactions are shown in Figure 5-6 and Figure 5-7, respectively. In addition, the energy-dependent standard deviations (%) are shown in Figure 5-8 for the C-graphite elastic scatter,  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$ ,  $^{238}\text{U}(n,\gamma)$  and  $^{239}\text{Pu}(n,\gamma)/^{239}\text{Pu}(n,\gamma)$  reactions. Both resonance absorbers ( $^{238}\text{U}$  and  $^{239}\text{Pu}$ ) have significant capture cross-section uncertainties (peak values of  $\sigma_{238\text{U}} = 47\%$  and  $\sigma_{239\text{Pu}} = 23\%$ ) between 10–2,000 eV, which corresponds to the large  $k_{\infty}$  sensitivities observed in Figure 5-7 for these reactions at these energies. In contrast to this relationship, a significant  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$  sensitivity in the thermal-energy region can be observed in Figure 5-6, although the  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$  standard deviation remains much smaller (<0.4%) and relatively flat across the energy range shown here.

It can also be seen in Figure 5-6 that the  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$  sensitivity on the  $k_{\infty}$  of the fresh fuel block (Ex. I-2a) is significantly larger at  $\sim 0.5$  eV compared with the  $k_{\infty}$   $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$  sensitivity of the depleted fuel block. For the burned fuel, the eigenvalue is  $\sim 50\%$  driven by  $^{239}\text{Pu}$  fission, so  $k_{\infty}$  is less sensitive to the  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$  reaction uncertainty, because it's only providing about 50% of the neutron multiplication in the system. There is also significant parasitic neutron absorption by  $^{239}\text{Pu}$  in the resonance region.

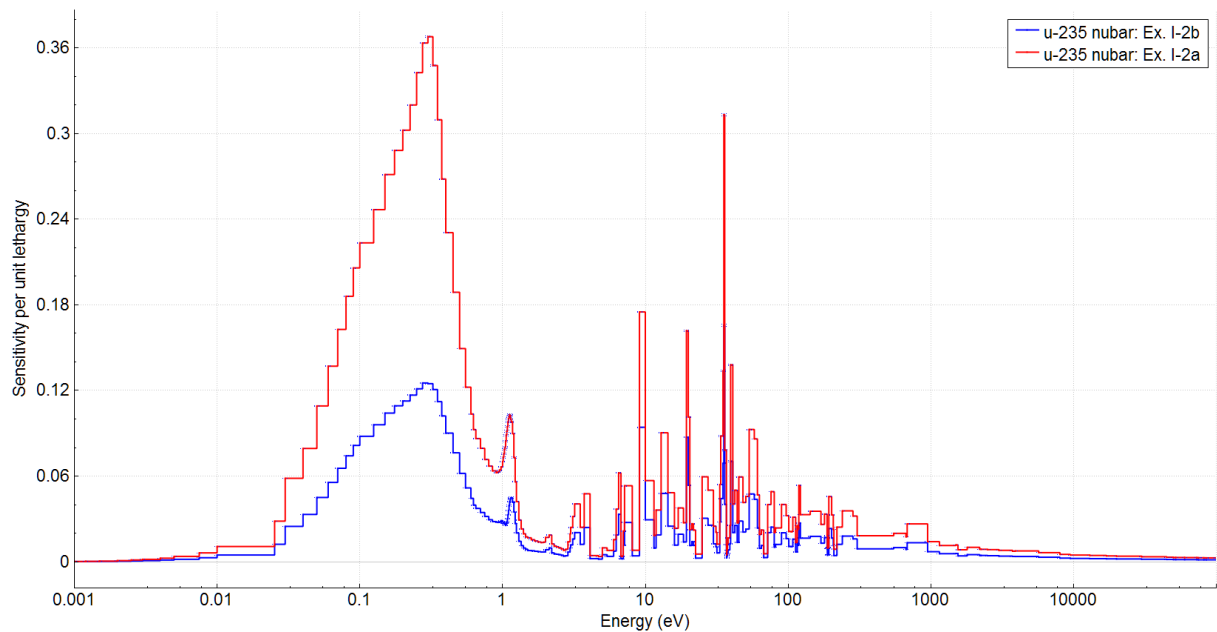


Figure 5-6. Ex. I-2a and I-2b  $k_{\infty}$  sensitivity profiles for the  $^{235}\text{U}(\bar{\nu})$  covariance matrices.

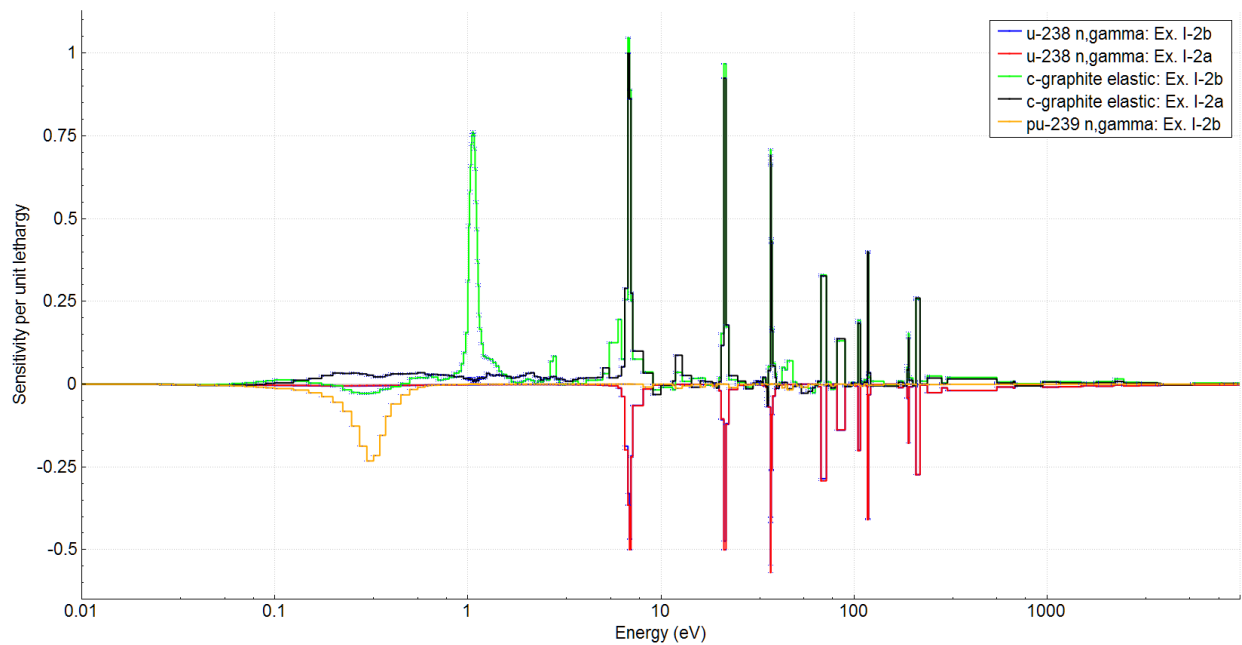


Figure 5-7. Ex. I-2a and I-2b  $k_{\infty}$  sensitivity profiles for the  $^{238}\text{U}(n,\gamma)$ ,  $^{238}\text{Pu}(n,\gamma)$  and C-graphite elastic-scatter covariance matrices.

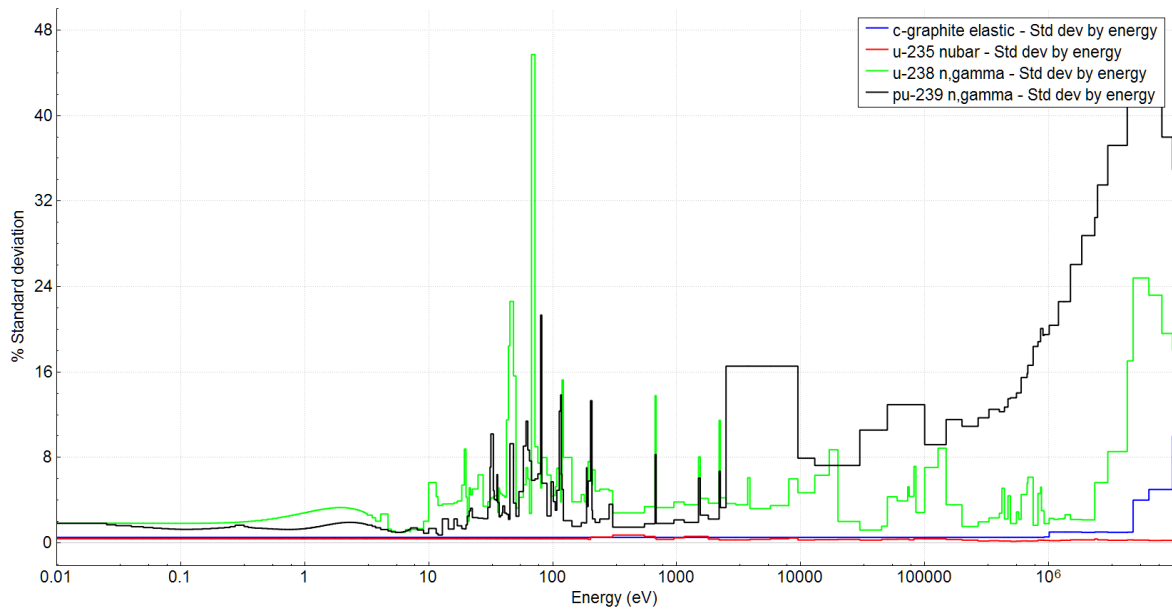


Figure 5-8. Standard deviation (%) of four nuclear data reactions as a function of energy.

The standard TSUNAMI energy-integrated sensitivity coefficients shown in Table 5-5 correspond to the % change in  $k_{\infty}$  for a 1% increase in the respective nuclide cross-section, applied over all energy groups. For example, a 1% increase in the Ex. I-2a  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction would lead to a 0.994% change in  $k_{\infty}$ , while the same change in the  $^{238}\text{U}(n,\gamma)$  cross-section would only change  $k_{\infty}$  by -0.171%. These integral sensitivity coefficients are *not* related to the ranking presented in Table 5-4. The integral sensitivity coefficients only consider the individual sensitivities per nuclide, assuming no interaction and full independence between the various cross-sections, according to the standard definition in TSUNAMI. It is interesting to note that according to the relative magnitude of the sensitivity coefficients shown in Table 5-5, the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction has the highest integral sensitivity coefficient for Ex. I-2b, but it does not feature in the top five individual covariance-matrix contributions in Table 5-4.

Table 5-5. TSUNAMI energy-integrated sensitivity coefficients for Ex. I-2a, I-2b and I-2c.

| Model | $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ | C-graphite (n,n') / C-graphite (n,n') | $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$ | $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$ |
|-------|---------------------------------------------------------|---------------------------------------|-------------------------------------------------------|---------------------------------------------------------|
| I-2a  | 0.994                                                   | 0.271                                 | -0.171                                                | -                                                       |
| I-2b  | 0.416                                                   | 0.373                                 | -0.172                                                | -0.151                                                  |
| I-2c  | 0.697                                                   | 0.484                                 | -0.180                                                | -0.084                                                  |

### Statistical NEWT/Sampler/RAVEN U/SA Results

In this section the Phase I Ex. I-2a, I-2b and I-2c results obtained with the NEWT/Sampler/ RAVEN sequence are discussed and compared with the TSUNAMI results. The three Sampler data sets consist of 1,000 NEWT perturbations each; an example of the results obtained for Ex. I-2a is shown in Figure 5-9. The 1,000 eigenvalues range over more than 3%, with the variances in the sample mean ( $\mu$ ) and standard deviation ( $\sigma$ ) decreasing with sample size up to approximately 300 samples, whereafter  $\sigma$  vary within a small 10 pcm band. The statistical-sampling approach and its indicators are associated with confidence intervals that depend on the size of the sample set. The confidence interval of the sample mean,  $\mu$ , is a function of the sample size,  $n$ , and the standard deviation,  $\sigma$ , and is given by Equation (5-1):

$$\mu_{\text{conf}} = \pm \frac{1.96 \sigma}{\sqrt{n}} \quad 5-1$$

For a sample size of 1,000 a 95% confidence interval<sup>26</sup> of  $\pm 0.0003$  (or 0.028% of the mean) is obtained for Ex. I-2a, so that  $\mu_{95} = 1.05077 \pm 0.00030$ . The relative 95% confidence interval of the standard deviation  $\sigma$  on a value of e.g. 0.50% would equal 0.0225%, so that  $\sigma_{95\%} = 0.500 \pm 0.023\%$ . Because these values are relatively small for a sample size of 1,000, the  $\sigma_{95\%}$  confidence intervals are not shown in the discussion that follows.

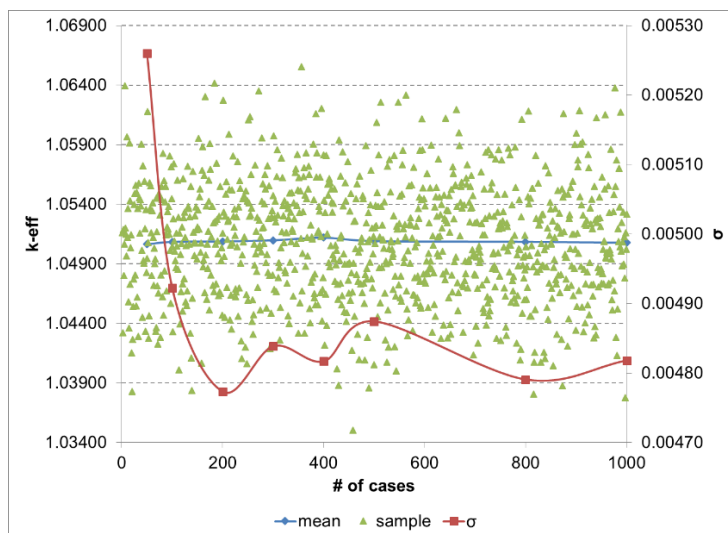


Figure 5-9. NEWT/Sampler results for Ex. I-2a: Sample mean ( $\mu$ ) and standard deviation ( $\sigma$ ) variance with sample size.

<sup>26</sup> A 95% confidence implies that for every time a set of 1,000 NEWT runs are repeated (assuming there were a very large number of perturbed Sampler files available), there will be another value for the mean  $\mu$  of the sample. For 95% of these sets of 1,000 runs each,  $\mu$  will be between  $\pm 0.0003$  from the respective mean values, but in 5% of the cases it will not be.

The statistical indicators calculated for the three sets of 1,000 NEWT samples, and a comparison of with the TSUNAMI data, are presented in Table 5-6 and Table 5-7, respectively. The  $k_{\infty}$  standard deviations of the three NEWT/Sampler perturbed cross-section sample sets ( $\sigma_{cov}$ ) vary between 0.44 and 0.53%, which agrees reasonably well with the respective TSUNAMI  $\sigma_{cov}$  values (0.50 and 0.54%). The CE KENO-VI  $k_{\infty}$  values is 1.0% higher than the 252-group NEWT mean  $k_{\infty}$  values for Ex. I-2a, which can be attributed to modeling differences discussed in Section 3.2.1. The TSUNAMI and Sampler results for the depleted and supercell fuel blocks are better matched compared to the fresh fuel block, but the difference between these cases is not seen as significant. The use of the larger and better-moderated Ex. I-2c supercell did not lead to a significant difference with the single fresh block  $\sigma_{cov}$  value, although the  $k_{\infty}$  of these two models differ by more than 1,200 pcm. The presence of additional resonance absorption by  $^{239}\text{Pu}$  caused an increase in  $\sigma_{cov}$  value of the Ex. I-2b depleted fuel block, with TSUNAMI predicting a slightly smaller increase (0.04%) between the fresh and depleted blocks compared to Sampler (0.07%), but this difference is likewise not seen as statistically significant.

Table 5-6. Ex. I-2a, Ex. I-2b and Ex. I-2c  $k_{\infty}$  NEWT/Sampler/RAVEN statistical indicators.

| Indicator                                              | Ex. I-2a     | Ex. I-2b     | Ex. I-2c     |
|--------------------------------------------------------|--------------|--------------|--------------|
| Nominal $k_{\infty}$                                   | 1.05059      | 0.96314      | 1.06332      |
| Mean $k_{\infty}$ ( $\mu \pm 95\%$ conf. int.)         | 1.05077 (30) | 0.96336 (32) | 1.06339 (29) |
| $\sigma_{cov}$                                         | 0.00482      | 0.00510      | 0.00470      |
| $\sigma_{cov}$ (%)                                     | 0.459        | 0.530        | 0.442        |
| $k_{\infty}$ 95 <sup>th</sup> percentile <sup>27</sup> | 1.05858      | 0.97231      | 1.07143      |

Table 5-7. Comparison of CE TSUNAMI and NEWT/Sampler  $k_{\infty}$  uncertainty.

| Model                                 | Ex. I-2a                  |                    | Ex. I-2b                  |                    | Ex. I-2c                  |                    |
|---------------------------------------|---------------------------|--------------------|---------------------------|--------------------|---------------------------|--------------------|
|                                       | $k_{\infty} \pm \sigma_s$ | $\sigma_{cov}$ (%) | $k_{\infty} \pm \sigma_s$ | $\sigma_{cov}$ (%) | $k_{\infty} \pm \sigma_s$ | $\sigma_{cov}$ (%) |
| CE TSUNAMI                            | 1.06101 (10)              | 0.502              | 0.96605 (9)               | 0.544              | 1.06332 (15)              | 0.510              |
| 252-g NEWT/Sampler                    | 1.05077 (30)              | 0.459              | 0.96336 (32)              | 0.530              | 1.06339 (29)              | 0.442              |
| Relative difference (%) <sup>28</sup> | 0.97                      | 8.57               | 0.28                      | 2.57               | -0.01                     | 13.33              |

As indicated in Section 4.4.2, RAVEN calculates linear-regression fit coefficients<sup>29</sup>; not the individual coefficient sensitivities as calculated by CE TSUNAMI. The RAVEN data can still be used, however, to obtain a relative ranking of the various nuclide cross-section reaction contributors, and this ranking can be compared with the relative ranking of the TSUNAMI sensitivity coefficients.

<sup>27</sup> The 95<sup>th</sup> percentile is the value below which 95% of the data may be found. The 97.72<sup>th</sup> percentile =  $\mu + 2\sigma$ .

<sup>28</sup> (TSUNAMI  $k_{\infty}$  – NEWT  $k_{\infty}$ ) / TSUNAMI  $k_{\infty}$

<sup>29</sup> See Appendix B-1 for the definitions of the RAVEN sensitivity and PCC parameters

In addition to the sensitivity coefficients, the RAVEN PCCs are used as a first screening to assess whether a significant degree of linear correlation exists between the cross-section reaction and the eigenvalue. PCC values larger than  $R^2 = 0.01$  are typically indicative of a meaningful degree of linear correlation, and the sensitivity coefficients determined by RAVEN can be used for a ranking assessment. On the other hand, PCC values less than 0.01 indicates weak or no linear-correlation dependencies, and the sensitivity coefficients can potentially contain larger uncertainties.

As an illustration of the PCCs, two scatterplots are shown in Figure 5-10 for the  $k_\infty$  obtained for Ex. I-2c as a function of the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  perturbation ( $Q_{x,g}$ ) factors in Sampler. The linear-regression  $R^2$  values are shown for Group 36 (5 eV) on the left and Group 42 (0.375 eV) on the right, and it can be seen that only the Group 42 value of 0.116 indicates a significant linear correlation between  $k_\infty$  and the  $^{239}\text{Pu}(n,\gamma)$  cross-section perturbation factors.

A comparison of the relative TSUNAMI and RAVEN sensitivity-coefficient rankings for four dominant nuclide cross-section reactions is shown in Table 5-8. In addition to the sensitivity coefficients, the table also includes PCCs for the three lattice cases. It can be seen in Table 5-8 that the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction is again ranked as the most important nuclear data uncertainty to the eigenvalue, as it was for the VHTRC (4.4.2). The ranking of the third-place  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  reaction is also the same between TSUNAMI and RAVEN, but RAVEN ranks the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  sensitivity higher than TSUNAMI. The reason for these differences in the less sensitive cross-section covariances cannot be identified without performing a larger number of samples (e.g. 10,000) to increase the confidence in the RAVEN sensitivity indices, which is currently not available in Sampler. As noted before, direct comparison between the TSUNAMI and RAVEN indices requires some caution, as the two sensitivity metrics differ substantially.

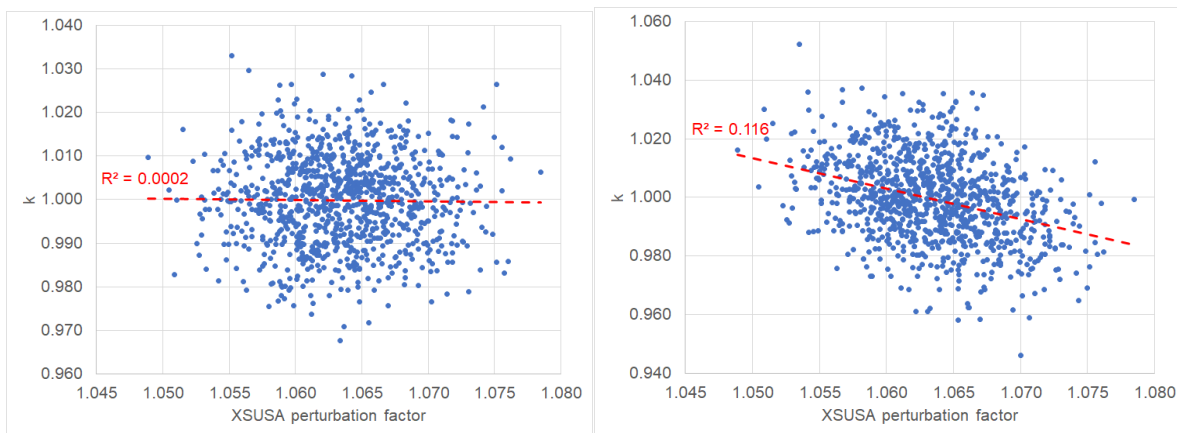


Figure 5-10. Ex. I-2c scatterplots of  $k_\infty$  vs.  $^{239}\text{Pu}(n,\gamma)$  cross-section perturbation factors for Group 36, left, and Group 42, right.

A few examples of the RAVEN sensitivity and PCC profiles for Ex. I-2a, 2b and 2c are shown Figure 5-11 and Figure 5-12, respectively, as a function of neutron energy (on a log scale). The impact of the  $^{238}\text{U}(n,\gamma)$  and  $^{239}\text{Pu}(n,\gamma)$  resonance structures can be observed in Figure 5-11, with the large peak in the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  sensitivity coefficient matching the trend shown in the TSUNAMI data for this reaction (Figure 5-7). The PCC for the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  reaction in Ex. I-2a is much smaller than the coefficients for Ex. I-2b and I-2c (Figure 5-12) and also lower than the typical PCC rule-of-thumb limit of 0.01, which indicates a weak dependency at best. The small sensitivity coefficient (less than 0.01 for most groups) could therefore be an artifact of higher uncertainties. A similar trend can be identified in Figure 5-12 for the C-graphite (n,n') / C-graphite (n,n') reaction, where Ex. I-2a exhibits inverse trends to Ex. I-2b and I-2c, but because the PCCs are so small for this reaction, the degree of linear correlation is weak, and a meaningful conclusion cannot be drawn from these data alone.

Table 5-8. Comparison of TSUNAMI and NEWT/Sampler/RAVEN  $k_\infty$  NSCs and PCCs for Phase I

[rank in brackets]

| Reaction                                                | I-2a       | I-2b       | I-2c       |
|---------------------------------------------------------|------------|------------|------------|
| CE TSUNAMI integral sensitivity coefficient             |            |            |            |
| $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ | 0.994 [1]  | 0.416 [1]  | 0.697 [1]  |
| C-graphite (n,n') / C-graphite (n,n')                   | 0.271 [2]  | 0.373 [2]  | 0.484 [2]  |
| $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$   | -0.171 [3] | -0.172 [3] | -0.180 [3] |
| $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$ | -          | -0.151 [4] | -0.084 [4] |
| NEWT/Sampler/RAVEN normalised sensitivity coefficient   |            |            |            |
| $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ | 0.167 [1]  | 0.347 [1]  | 0.687 [1]  |
| C-graphite (n,n') / C-graphite (n,n')                   | 0.030 [3]  | 0.030 [4]  | 0.037 [4]  |
| $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$   | -0.035 [2] | -0.067 [3] | -0.069 [3] |
| $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$ |            | -0.188 [2] | -0.115 [2] |
| Pearson Correlation Coefficient                         |            |            |            |
| $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ | 0.080 [1]  | 0.265 [3]  | 0.577 [1]  |
| C-graphite (n,n') / C-graphite (n,n')                   | 0.062 [2]  | 0.055 [4]  | 0.079 [4]  |
| $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$   | -0.071 [3] | -0.318 [2] | -0.338 [3] |
| $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$ | -          | -0.524 [1] | -0.342 [2] |

### 5.3 Conclusion

The focus of this chapter was the generation of suitable lattice models that can be used to construct the perturbed P/R core models, utilizing the NEWT/Sampler statistical U/SA sequence described in Chapter 2. RAVEN was applied to determine the uncertainty metrics and energy-dependent sensitivity and PCCs. The NEWT/Sampler calculations all used a sample size of 1,000 to ensure the best possible statistics currently available within the limitations of SCALE.

The  $k_{\infty}$  relative standard deviations due to the cross-section covariance data varied between 0.50–0.54% for the three lattice models Ex. I-2a, I-2b and I-2c (Table 5-4). In terms of the nuclide covariance-matrix contributors to the uncertainty in  $k_{\infty}$ , the largest Ex. I-2a contributor was found to be the covariance for the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction, followed by the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  (radiative capture) reaction. The Ex. I-2b depleted fuel block  $k_{\infty}$  uncertainty contributors also include the capture and fission reactions from the resonance absorber  $^{239}\text{Pu}$ , and for all three lattice cells the C-graphite  $(n,n') / \text{C-graphite } (n,n')$  reactions contribute significantly to the uncertainty in  $k_{\infty}$ .

## CHAPTER 5: MHTGR-350 EXERCISE I 1: LATTICE NEUTRONICS

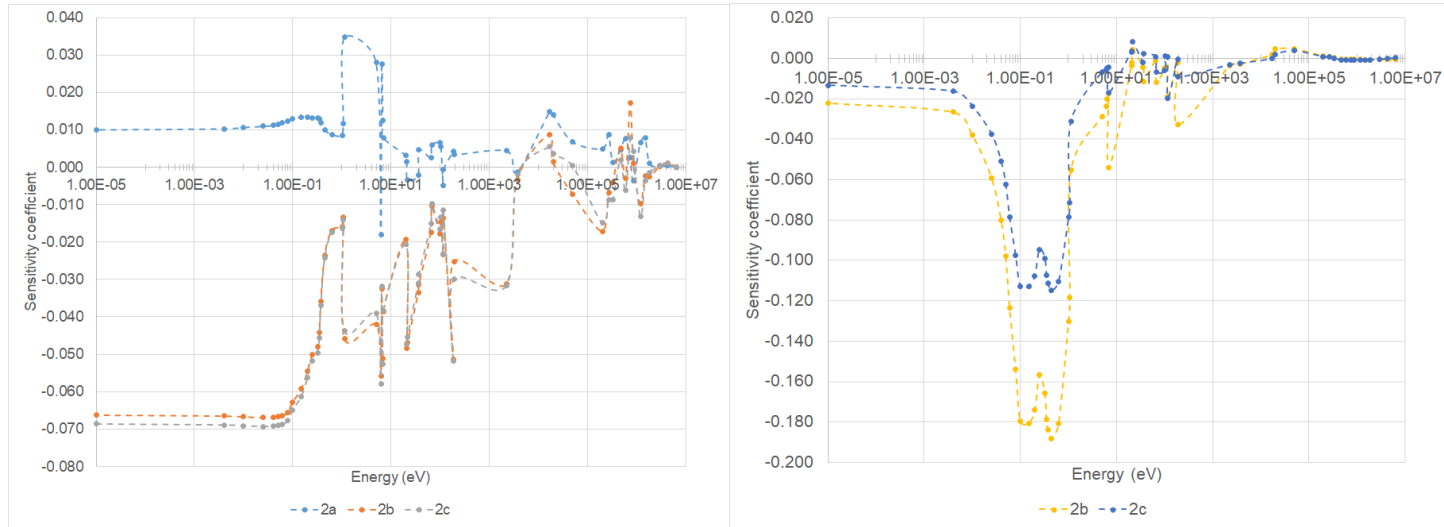


Figure 5-11. RAVEN sensitivity profiles for the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  (left) and  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  (right) cross-section reactions.

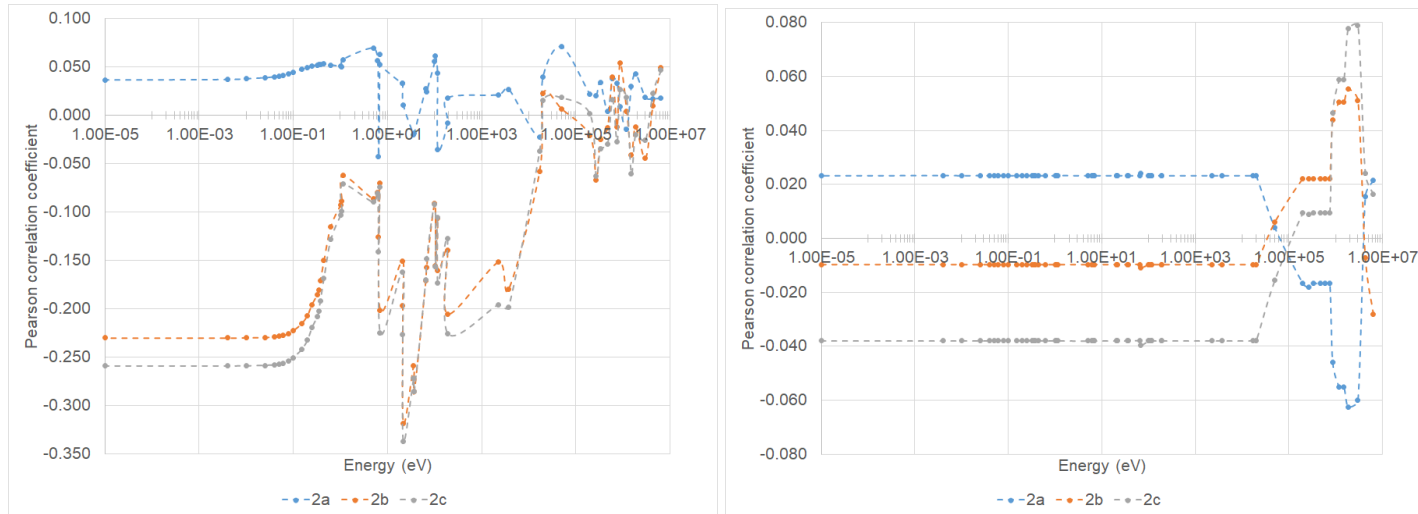


Figure 5-12. RAVEN Pearson Correlation Coefficients for the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  (left) and C-graphite (n,n') / C-graphite (n,n') (right) cross-sections as a function of energy.

## 6. MHTGR-350 EXERCISE II-2: STAND-ALONE STEADY-STATE CORE NEUTRONICS

*“I have approximate answers, and possible beliefs, and different degrees of uncertainty about different things, but I am not absolutely sure of anything.” Richard Feynman.*

The focus of this chapter is on the propagation of cross-section uncertainties from the Phase I lattice models to the stand-alone neutronics Phase II P/R core models, using the NEWT/Sampler statistical U/SA sequence described in Chapter 2. Exercise II-2, as defined in Section 4.1, consist of two subcases that assess the impacts of cross-section uncertainties without feedbacks from changes in the fuel and graphite temperatures.

The results obtained for Exercise II-2 is reported in Section 6.2, as shown on the left of Figure 6-1. A single fixed isothermal fuel and graphite temperature of 1,200 K is used for the entire RELAP5-3D model; i.e. no perturbed RELAP5-3D models are coupled with the perturbed PHISICS neutronics models in this stand-alone neutronics sequence. The grey box in the left section of Figure 6-1 points to a possible CRW transient case that uses the Exercises II-2 steady-state to perform a CRW with no thermal feedback. Such an event can be used to isolate the contributions of cross-section and kinetic uncertainties, but without temperature feedback, the rise in power will not be countered. This CRW option is not included in this work, since it is of lesser importance to HTGR designers interested in the fully coupled behaviour of the HTGR core, and also because the focus of this dissertation is the U/SA of the interaction between thermal fluids and neutronics.

The U/SA of a fully coupled CRW transient is explored in Section 7.3, as indicated on the right of Figure 6-1. Figure 6-1 also includes an overview of the subsequent sequences defined for Phases II–IV, as well as the relevant sections where the U/SA results are reported in this work. The stand-alone thermal fluids Exercise II-4 (using as single fixed power profile) is discussed in Section 7.4, followed by a series of perturbed PLOFC transients based on these perturbed steady-states in Section 7.5. The coupled steady-state (Exercise III-1) reported in Section 8.1 is used as a basis to assess the impact of both cross-section and thermal fluid uncertainties on the CRW transient (Exercise IV-2) in Section 8.2.

A possible PLOFC sequence with coupled feedback is indicated in grey as part of the Phase-IV options; but due to the significant calculation effort required to run a coupled P/R model of a subcritical transient, this option is not pursued further as part of this work. The differences between these various combinations of neutronics and thermal fluid perturbed models is further highlighted in Figure 6-2.

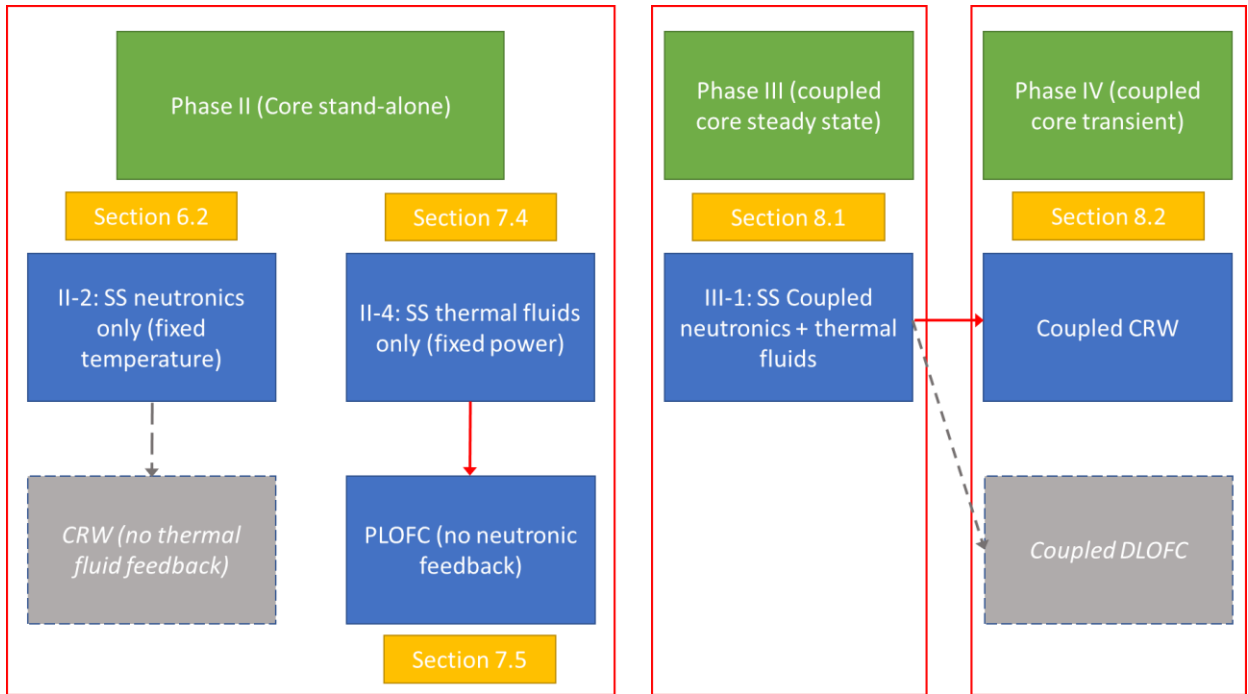


Figure 6-1. Calculation flow for the MHTGR-350 Phase II-IV Exercises

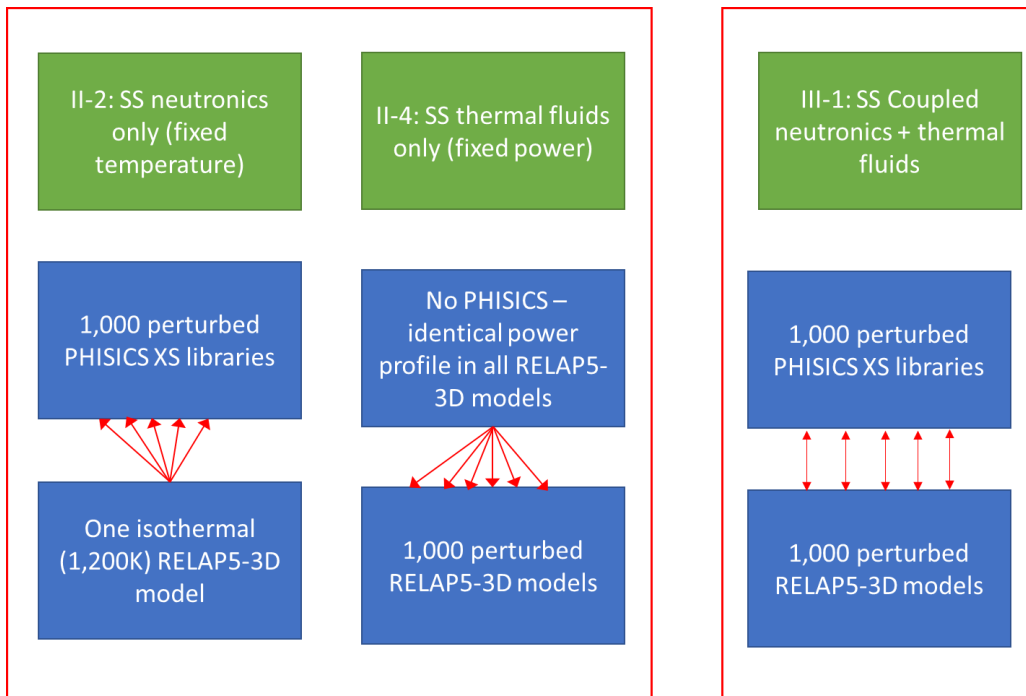


Figure 6-2. Steady-state coupling options of perturbed PHISICS and RELAP5-3D models.

## 6.1 Specification of the IAEA CRP on HTGR UAM Stand-Alone Neutronics Core Cases

Two full-core steady-state neutronics calculations at HFP conditions is defined using the given fresh (Exercise II-2a) and mixed (Exercise II-2b) core number densities, respectively. A representation of the 1/3<sup>rd</sup> core layout is shown in Appendix A Figure A-3. For Exercise II-2a, a core model consisting of fresh fuel is constructed using the few-group cross-section library created in Exercise I-2a.

The fresh-core model uses the same fresh fuel-block cross-section library and isotopics in all 22 fuel locations and ten axial layers (220 in total). There are no radial or axial variations in the composition or cross-section representation of the fuel and reflector blocks, and the control rods are fully withdrawn from the core. The data required to construct the core model—e.g. fuel and reflector block dimensions and isotopics—are listed in Appendix A.

Propagation of cross-section uncertainties from the lattice models (Exercises I-2a, b, and c) to the core models (Phase II) is achieved by using the libraries generated in Phase I in the Phase II core models. Methodological uncertainties, which are associated with methods and modeling approximations utilized in lattice physics codes are beyond the scope of this work. Two core-loading patterns will be analysed for Phase II of the CRP:

- Exercise II-2a: The first case is a fresh core at HFP conditions and with no control rods inserted. This core is identical to the starting point of Exercise II-1b. The cross-section libraries assigned to the fresh fuel blocks should be generated using the Exercise I-2a fresh fuel-block lattice model to propagate the cross-section covariance data from Phase I to Phase II. The use of a periphery supercell for the fresh core or a single fresh cross-section library assigned to all 220 fresh fuel blocks is investigated in this work. This fresh-core model will not be used in subsequent phases.
- Exercise II-2b: The second core will be used for the transients defined in Phase IV. A mixed core at HFP conditions is constructed using alternating fresh and depleted fuel blocks in the pattern shown in Figure A-4. The control-rod worth is determined by withdrawing the control rods from their nominal location in the first two fuel blocks to the bottom of the first top reflector block (equal to 158.6 cm). The most-basic version of this exercise uses the fresh and depleted single-block isotopic-composition definitions and cross-section libraries, and no supercells at the core periphery.

## 6.2 Phase II Exercise II-2: Core Stand-Alone Neutronics Results

The choice of the lattice cell for the generation of HTGR few-group cross-sections for use in steady-state and transient core models is an important contributor to modeling uncertainties. In the case of prismatic HTGR designs, the cross-section libraries were historically generated using a single “representative” fuel block at various temperature points, but it was found that the radial core power density in the MHTGR-350 core can be affected by as much as 10% when a supercell lattice approach is used (Rouxelin et al. 2018). The nominal results summarized in Section 3.3.1 were obtained in the 2016–2017 period at INL by Pascal Rouxelin and the author as part of the joint NCSU/INL contributions to the IAEA CRP on HTGR UAM. In addition to the journal publication referenced above, the nominal results were also reported in an INL report (Rouxelin and Strydom 2016) and Rouxelin’s Ph.D. dissertation (Rouxelin 2019). Because the nominal results were extensively reported in the three listed references, only a high-level summary will be provided here.

The main purpose (and contribution) of this section is the propagation of the cross-section uncertainties into the Phase II P/R core models using the statistical NEWT/Sampler sequence described in Chapter 2. RAVEN was again used to provide sensitivity indices for selected figures of merit. A subset of the Phase II stand-alone U/SA results was reported by the author at the HTR-2018 conference (Strydom et al. 2018).

### 6.2.1 Exercises II-2a and II-2b Definitions and Models

In the standard SCALE code sequence, the neutron-flux spectrum is used as a weighting function to prepare self-shielded-nuclear data, and with those data, the collapsed cross-section libraries (Williams 2011). In this work, the TRITON-NEWT (T-NEWT) modules of SCALE 6.2 was used to collapse<sup>30</sup> the 252-group lattice-cell fluxes into 26-, 8- and 2-group libraries<sup>31</sup> for use in the Phase II–IV steady-state and transient P/R core models (the 2-group models are only used in Chapter 8 for the transient analysis). Serpent2 and KENO-VI were used to generate reference eigenvalues and spectra for comparison with the NEWT results, and the P/R “ring” model, developed for the MHTGR-350 benchmark (Strydom et al. 2015), was used to provide a fixed isothermal temperature of 1,200 K to PHISICS<sup>32</sup>. An alternate approach would have been to use PHISICS in stand-alone mode, i.e. without coupling to RELAP5-3D, but because one of the objectives of this work was to minimize model-uncertainty effects, the same P/R model was used for the core stand-alone and coupled results reported in Chapters 4 and 5.

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<sup>30</sup> Detail on the cross-section preparation is provided in Appendix B-4.

<sup>31</sup> See Table 2-4 for the energy group boundaries and a discussion of the 26- and 8-group structures.

<sup>32</sup> More detail on the RELAP5-3D “ring” MHTGR-350 model is provided in Appendix B-1.

Because PHISICS is considered a subroutine of the coupled PHISCS/RELAP5-3D code, the RELAP5-3D component was used as a “driver-wrapper” in for Exercise II-2a/2b. PHISICS uses a hexagonal mesh for the neutronics solution corresponding to a fuel or reflector block, as shown in the core layout in Figure 6-3. One third of the core is modeled to make use of the 120 degree azimuthal symmetry, and power densities are generated for each fuel block (e.g. 10 axial levels of 22 blocks each). For the RELAP5-3D “ring” model temperatures, these block-power values are homogenized into three rings (also Figure 6-3). The ring model follows the common system-code homogenization approach of modeling the inner reflector, fueled core region, and outer reflector as rings in cylindrical coordinates, with three additional rings representing the core barrel, the RPV, and outer air boundary layer.

The 220 power-density values provided by Intelligent Nodal and Semi Structured Treatment for Advanced Neutron Transport (INSTANT) are therefore reduced for RELAP5-3D to 30 (three rings with 10 levels each). As an example of the homogenization scheme, consider the Fuel Ring 1 (FR1) Blocks 8–13 in Figure 6-3. PHISICS calculates the power generation for each of these blocks based on the homogenized cross-sections provided by the NEWT sequence at the specific temperature points provided by RELAP5-3D. The power is then homogenized over all six blocks in FR1 (and eight blocks each for FR2 and FR3) on each axial level, so that the power on the first axial level of FR1 is given as the total homogenized value of Blocks 8–13 on Core Level 1. This “Ring 1, Level 1” power source is subsequently passed on to RELAP5-3D as input to the next temperature calculation, which is also determined for the homogenized FR1 because RELAP5-3D cannot simulate individual hexagonal blocks.

The ring-averaged temperature<sup>33</sup> is passed back to PHISICS as a two-temperature feedback component for fuel (Doppler) and moderator temperatures, which are used by the cross-section interpolation routine to construct the updated values of the cross-sections from the cross-section library tabulated at 300, 900, and 1500 K. In summary, PHISICS therefore produces 220 ( $22 \times 10$ ) homogenized block powers, which are volume-averaged within RELAP5-3D to 30 ring powers ( $3 \times 10$ ) to match the 30 fuel and moderator ring temperatures. The maximum values of these fuel temperature and power spatial values are designated as the Maximum Fuel Temperature (MFT) and maximum power, respectively.

The focus in this work is on the active-core region (e.g. Blocks 8–21, 23–26, and 28–31; or Rings 4–6) because the FOMs are eigenvalues and power densities, and there is no power generation outside the active-core region (i.e. no non-local heat). Two variants of the stand-alone core-neutronics core exercises were defined in the Phase II specifications:

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<sup>33</sup> The RELAP5-3D model is described in Appendix B-1.

**Exercise II-2a:** A fresh core at HFP conditions and with no control rods inserted (top of Figure 6-4). The specifications allowed two representations of the lattice cross-sections: fresh fuel blocks libraries that are generated from the Exercise I-2a fresh fuel block NEWT lattice models (Section 3.2), as well as the addition of a periphery supercell if desired.

**Exercise II-2b:** The mixed core at HFP conditions, shown at the bottom of Figure 6-4, will be used for the coupled core cases defined in Phases III and IV. The control rods are also added to Block 33 in Figure 6-3. The homogenized Block 33 “rodded” cross-section data set was determined from the OECD Benchmark specifications and allows an assessment of the impact of cross-section uncertainties on the control-rod worth to be performed. The control-rod worth is determined by withdrawing the Block 33 control rods from their nominal location in the first two fuel blocks to the bottom of the first top reflector block (158.6 cm).

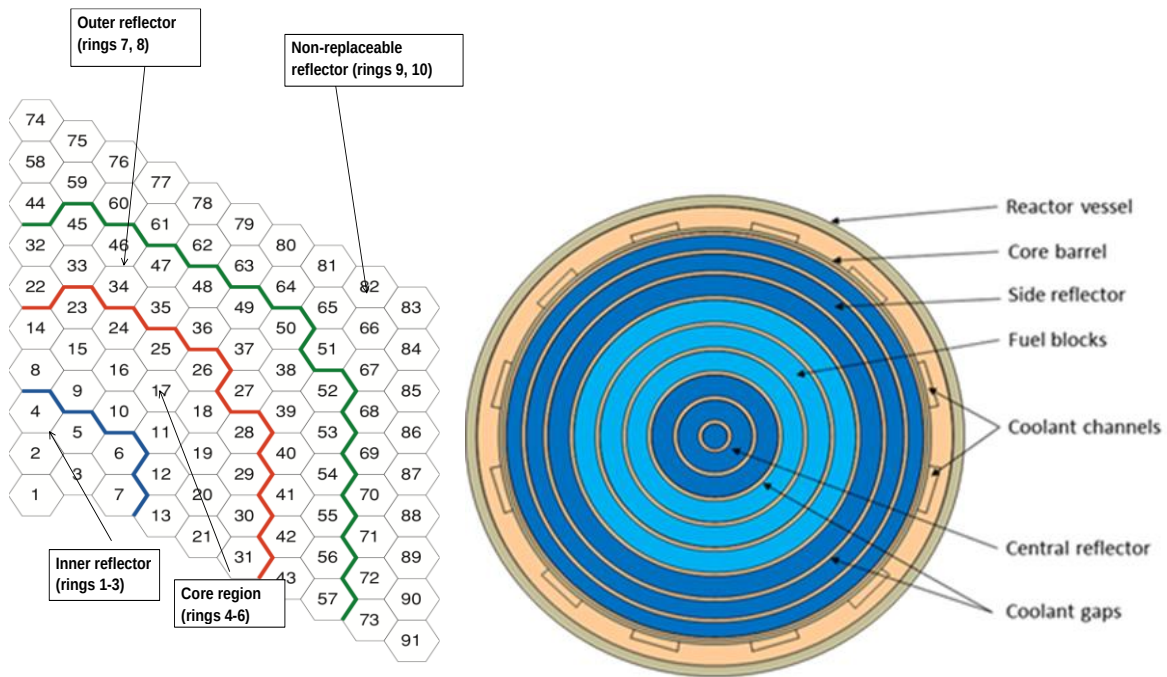


Figure 6-3. MHTGR-350 core numbering layout and RELAP5-3D “ring” model radial representation.

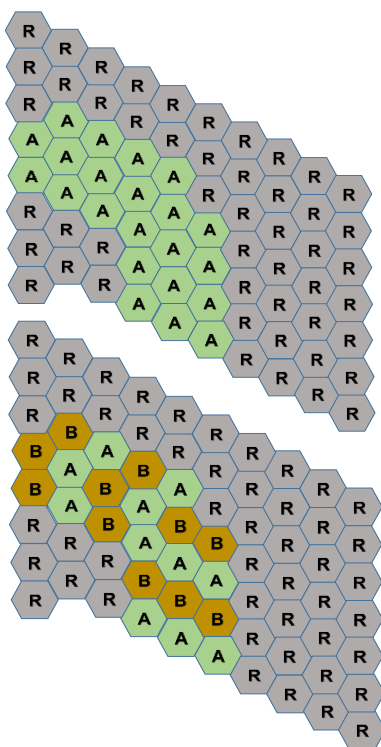


Figure 6-4. Ex. II-2a fresh (top) and II-2b mixed (bottom) cores with (A) fresh fuel, (B) depleted fuel, and (R) reflector blocks.

### 6.2.2 Exercise II-2a and II-2b Uncertainty Results

Based on the geometrical layout of the MHTGR-350 core shown in Figure 6-4, a total of 15 supercells were investigated in terms of spectrum across the central block, relative fluxes, and power densities (Rouxelin and Strydom 2016). In Figure 6-7, four options are shown for a fresh fuel block located at various locations along the core periphery (Cells  $k$ ,  $l$  and  $m$ ) or the core center (Cell  $i$ ), as well as a reflector block next to the fuel region (Cell  $r$ ) (Rouxelin, et al. 2018).<sup>34</sup> Similar cells can be constructed for the mixed-core load pattern. Neutron flux and cross-sections are generated for the heterogeneous central block of the supercell, shown as striped pink blocks in the figure. The solid pink blocks are homogenized to obtain a representative spectrum around the central block. The addition of more graphite blocks in the supercell softens the neutron spectrum experienced by the central fuel block, as shown in Figure 6-6. The simplest P/R core model for Ex. II-2a consists of identical fresh fuel everywhere in the core region, based on the 252-group libraries created for the single fresh block defined in Ex. I-2a. The fuel blocks are surrounded by identical reflector blocks based on 252-group libraries created from the reflector Supercell  $r$  (Figure 6-5). This option is shown on the left of Figure 6-7.

<sup>34</sup> Due to space limitations and the focus of these publications on nominal results only, the results of the 2016 and 2018 supercell studies will not be reported here; the interested reader is referred to the listed references.

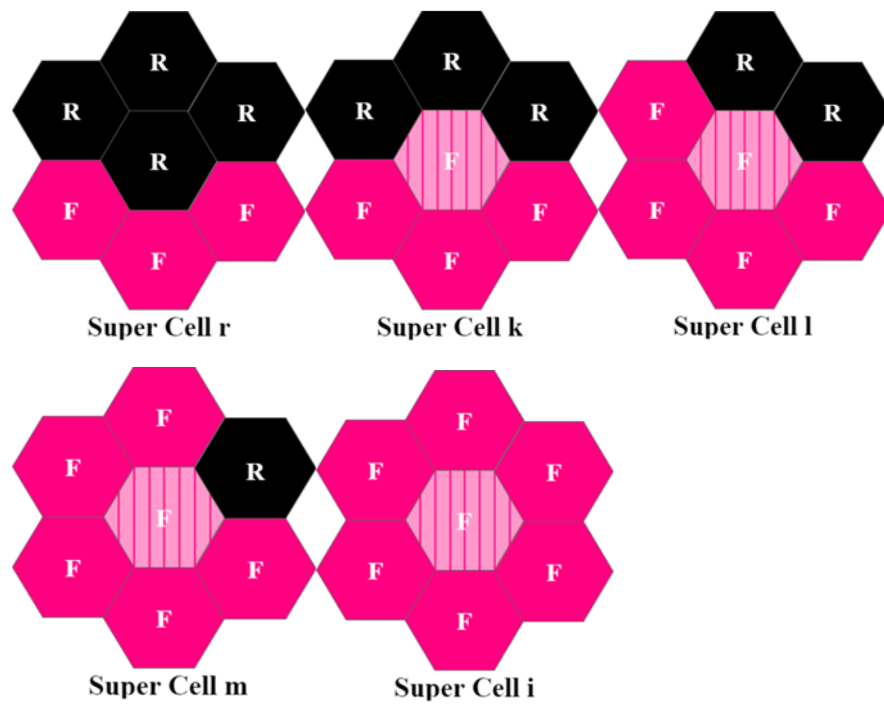


Figure 6-5. Fresh-core Supercells *k*, *l*, *m*, *i* and *r* (Rouxelin et al. 2018)

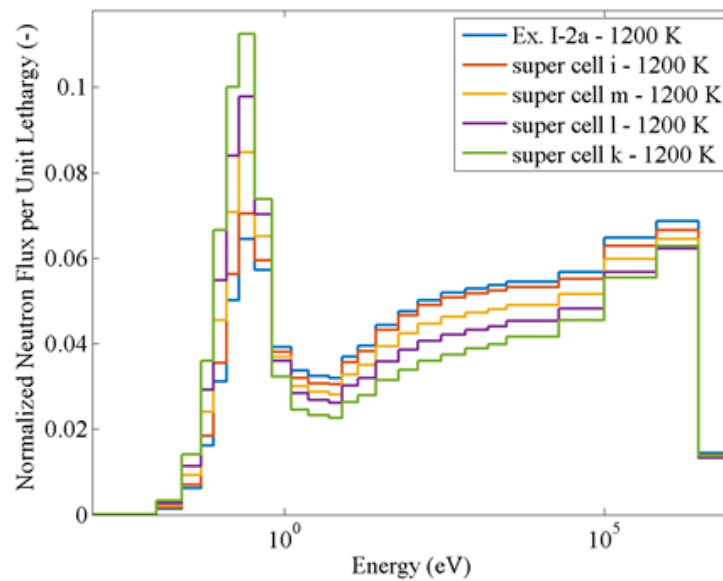


Figure 6-6. Normalized neutron flux per-unit lethargy in 26-group structure for Ex. I-2a and Ex. I-2c Supercells *i*, *m*, *l* and *k* (Rouxelin et al. 2018)

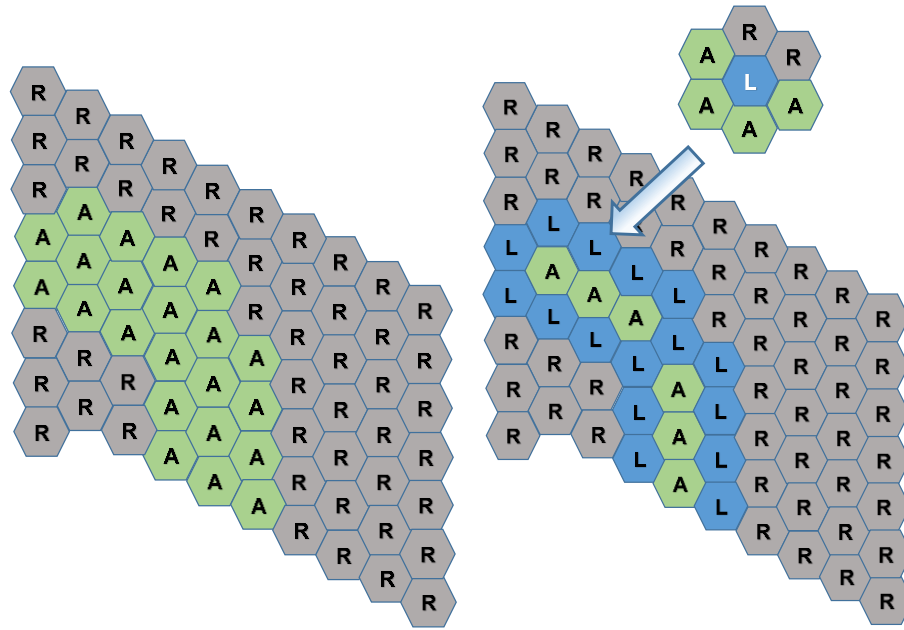


Figure 6-7. Use of supercell L for generation of fresh fuel block cross-sections in the fresh-core peripheral region. Core-2a-r (left) and core-2a-l-r (right) shown.

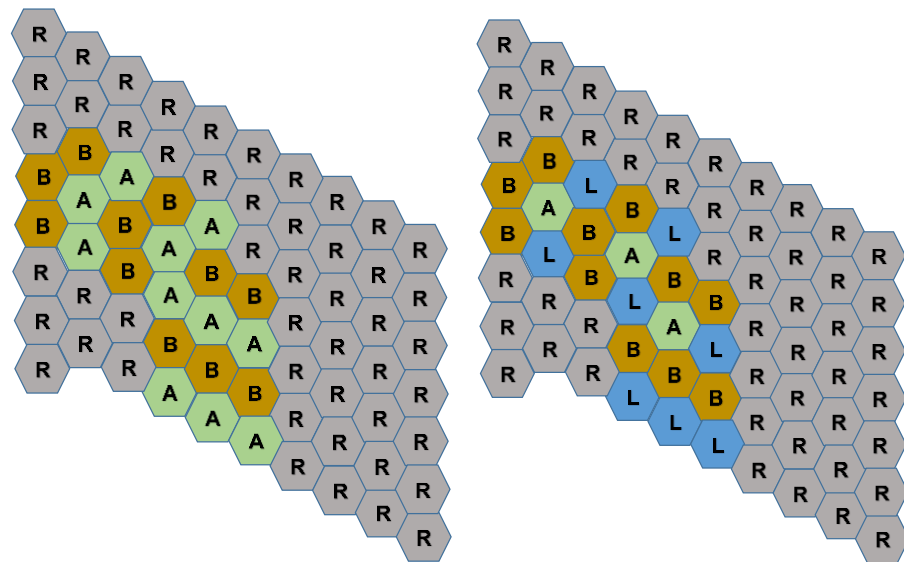


Figure 6-8. Use of supercell L for generation of fresh fuel block cross-sections in the mixed-core peripheral region. Core-2a-2b-r (left) and core-2a-2b-r-l (right) shown.

Due to the computational expense of generating perturbed cross-section libraries for all 15 supercell variants (i.e. each new cell requires 1,000 NEWT calculations), and the focus on uncertainty propagation rather than best-estimate nominal results in this study, it was decided to include only Supercell *l* as an example of the impact of a supercell lattice on the U/SA FOMs.

This library was used for all the fresh fuel blocks at the core periphery, as shown on the right side of Figure 6-7. A similar approach was taken for the mixed-core P/R model defined for Ex. II-2b (Figure 6-8).

The four fresh and mixed-core models described here are referred to as Core 2a, Core 2a-l-r, Core 2a-2b, and Core 2a-2b-l-r in the discussion that follows. The rodded versions of these models are designated with an additional R (e.g. 2a-2b-rR). The eight models are all rodded (R) and unrodded (r) variants of either the Exercise II-2a fresh core (i.e., Core 2a-r, Core 2a-rR, and Core 2a-l-r) or the Exercise II-2b mixed core (i.e. Core 2a-2b-r, Core 2a-2b-l-r, and their rodded versions). The “l” designation adds the peripheral cell model to the cross-section set. Although not specifically defined in the benchmark specifications, a core consisting of just burned fuel (i.e. Core 2b-r) has also been included here to quantify the differences caused by the addition of actinides.

The integral (scalar) FOMs are discussed first, consisting of the core eigenvalue ( $k_{eff}$ ), the axial offset (AO), and the power peaking (PP) values. In the case of core power, the AO is defined as the ratio of the power generated in the top half of the core to the total power (see Equation 6-3).

A perfect cosine axial-power shape would result in AO values close to zero.

$$AO = \frac{P_{top} - P_{bottom}}{P_{top} + P_{bottom}} \quad (6-3)$$

The PP is defined as the ratio of the core maximum-to-average power:

$$PP = \frac{P_{max}}{P_{avg}} \quad (6-4)$$

The AO and PP data can be used as indicators of changes in the axial distribution of spatial variables such as the power, xenon concentration, and temperature in the core region. However, because these two parameters are less meaningful for the neutronics stand-alone case without temperature feedback, the main focus of the discussion will be on the core eigenvalues.

In addition to the scalar parameters, the changes in the spatial power distributions are discussed in Section 3.3.2.4. The power generated in a specific mesh location contains the effects of all cross-section perturbations and is more concise to present than the 8-group fluxes or individual reaction rates.

### ***Integral Parameters Uncertainties: Eigenvalue, Axial Offset and Power Peaking***

A summary of the P/R sample mean ( $\mu$ ) and standard deviation ( $\sigma$ ) values obtained for the eight core models are presented in Table 6-1. The standard deviations are shown in both absolute and relative (to the mean in %) units, and the data set includes the core eigenvalue ( $k_{eff}$ ), AO, and PP parameters. As a first check, the values obtained for the NEWT/Sampler Ex. I-2a cases (Table 5-6) can be compared with the corresponding fresh-core 2a-r P/R results.

## CHAPTER 6: MHTGR EXERCISE II 2: STAND-ALONE STEADY-STATE CORE NEUTRONICS

Although the addition of the reflectors in the P/R core model leads to significant additional reactivity (1.06439 vs. 1.05077) due to thermalization of fast neutrons and backscatter into the core<sup>35</sup>, the  $\sigma$  values of the two sample sets are very similar (0.497 vs. 0.459%, respectively). An even closer match is obtained for the P/R core with depleted fuel everywhere (core 2b-r) and Ex. I-2b: 0.53% vs. 0.51%. The impact of cross-section covariances are therefore very similar in both the NEWT lattice and P/R core models, indicating the propagation of the cross-section uncertainties through the lattice libraries is a feasible U/SA methodology.

Table 6-1. P/R mean and standard deviation values for eight core models (sets of 1,000 each).

| Case    | FOM       | Metric         |                |              |                             |                       |          |          |
|---------|-----------|----------------|----------------|--------------|-----------------------------|-----------------------|----------|----------|
|         |           | Mean ( $\mu$ ) | $\sigma$ (abs) | $\sigma$ (%) | 95 <sup>th</sup> percentile | Variation coefficient | Kurtosis | Skewness |
| 2a_r    | $k_{eff}$ | 1.06439        | 0.00529        | 0.497        | 1.07289                     | 0.00497               | -0.25    | 0.01     |
|         | AO        | -0.01294       | 0.00227        | -17.536      | -0.00916                    | -0.17536              | 0.89     | -0.01    |
|         | PP        | 1.38201        | 0.00148        | 0.107        | 1.38444                     | 0.00107               | 0.12     | 0.02     |
| 2a_rR   | $k_{eff}$ | 1.06353        | 0.00529        | 0.498        | 1.07202                     | 0.00498               | -0.24    | 0.01     |
|         | AO        | 0.07207        | 0.00506        | 7.017        | 0.07642                     | 0.07017               | 50.98    | 2.92     |
|         | PP        | 1.44952        | 0.00148        | 0.102        | 1.45161                     | 0.00102               | 10.74    | 1.00     |
| 2a_lr   | $k_{eff}$ | 1.05317        | 0.00522        | 0.496        | 1.06141                     | 0.00496               | -0.06    | 0.03     |
|         | AO        | -0.01293       | 0.00230        | -17.800      | -0.00929                    | -0.17800              | 1.14     | 0.18     |
|         | PP        | 1.37167        | 0.00157        | 0.115        | 1.37438                     | 0.00115               | 0.07     | 0.20     |
| 2a_lrR  | $k_{eff}$ | 1.05216        | 0.00523        | 0.497        | 1.06054                     | 0.00497               | -0.24    | 0.01     |
|         | AO        | 0.07166        | 0.00632        | 8.813        | 0.07632                     | 0.08813               | 70.90    | -3.29    |
|         | PP        | 1.43835        | 0.00160        | 0.111        | 1.44062                     | 0.00111               | 12.62    | 0.54     |
| 2b_r    | $k_{eff}$ | 1.02069        | 0.00521        | 0.510        | 1.02959                     | 0.00510               | -0.04    | 0.11     |
|         | AO        | -0.01979       | 0.00158        | -7.990       | -0.01710                    | -0.07990              | 0.68     | -0.22    |
|         | PP        | 1.36978        | 0.00206        | 0.150        | 1.37329                     | 0.00150               | 0.08     | -0.05    |
| 2ab_rR  | $k_{eff}$ | 1.04249        | 0.00462        | 0.443        | 1.05029                     | 0.00443               | -0.10    | 0.09     |
|         | AO        | 0.08017        | 0.00564        | 7.034        | 0.08595                     | 0.07034               | 22.08    | -1.77    |
|         | PP        | 1.44753        | 0.00153        | 0.106        | 1.44996                     | 0.00106               | 3.21     | -0.02    |
| 2ab_lr  | $k_{eff}$ | 1.03734        | 0.00459        | 0.443        | 1.04508                     | 0.00443               | -0.10    | 0.09     |
|         | AO        | -0.01626       | 0.00159        | -9.802       | -0.01347                    | -0.09802              | 1.91     | 0.34     |
|         | PP        | 1.36571        | 0.00178        | 0.130        | 1.36863                     | 0.00130               | 0.32     | -0.21    |
| 2ab_lrR | $k_{eff}$ | 1.03640        | 0.00458        | 0.442        | 1.04418                     | 0.00442               | -0.10    | 0.09     |
|         | AO        | 0.08070        | 0.00620        | 7.678        | 0.08618                     | 0.07678               | 23.09    | 1.43     |
|         | PP        | 1.43877        | 0.00166        | 0.115        | 1.44132                     | 0.00115               | 4.91     | 0.79     |

<sup>35</sup> The P/R nominal eigenvalue of a bare fresh core (i.e. without reflectors) is within 21 pcm of the NEWT nominal case for a single fresh block. A very good agreement therefore exists between the lattice and core transport codes and models.

**Eigenvalue:** It can be seen in Table 6-1 that the core  $k_{\text{eff}}$  mean values vary significantly (more than 4%) between the depleted (2b-r) and fresh cores (2a-r), with the mixed cores containing both fuel types between these two extremes (Figure 6-9, left). The main observation from Table 6-1 is that, in contrast to these large  $k_{\text{eff}}$  differences, the standard deviations only vary between 0.44 and 0.51% (or 458–510 pcm), as shown in (Figure 6-9, right). This is a relatively tight uncertainty band for cores containing different fuel-loading patterns, rodged and unrodged reflector blocks, and peripheral supercell cross-section libraries. Figure 6-9 clearly shows that the  $k_{\text{eff}}$  uncertainties caused by cross-section data uncertainties are mostly insensitive to the spectral environment (e.g. when the rodged and unrodged core standard deviations are compared, or the cores using the Supercell I).

In addition, the uncertainties observed for the Phase II models are very similar to the uncertainties calculated for the Phase I lattice models (0.50–0.54%), indicating that the propagation of the 252-group NEWT/Sampler cross-section covariance data into the 26-group P/R model preserved the implicit uncertainty information within the 1,000 perturbed core libraries.

There is also a notable trend that the two single-fuel type core variants (e.g. 2a-r, 2a-l-r, and 2b-r) produced higher standard deviations than the mixed-core variants. This is interesting in the sense that the mixing of the two fuel types actually seems to decrease the impact of cross-section uncertainties slightly, possibly due to competing production/removal processes in the uranium, plutonium, and graphite isotopes when the underlying cross-sections are varied simultaneously, as well as the spectral changes that occur.

**Axial Offset:** Of the three FOMs included in this section, the AO shows the highest standard deviations (up to -18%, as shown in Figure 6-10). This is partly a function of the very small AO mean values, which are all lower than 0.09. Small perturbations in the axial-power profile would therefore result in relatively large percentage variances. It can also be seen from these two figures that the standard deviations are the largest for the smallest mean values in an inverse relationship. The largest standard deviations occur for the rodged cores, which pushed the power profile lower and resulted in negative AO values (i.e. more power is generated in the lower region of the core than the top region).

The cross-section data uncertainties, therefore, had a significant impact on the AO uncertainties (at least in percentage terms), but it is shown in Chapter 5 that this trend is limited to these (artificial) isothermal core models with their cosine axial-power shapes.

The low AO values for all the cores (some of which are negative) indicates that the axial-power production in the upper and lower regions of the core is almost equal (i.e. close to a classical cosine power profile). This is unusual for an HTGR core, which usually is associated with top-peaked axial-power distributions.

The PP generated in the fresh and depleted cores occurs in the outer fuel ring (e.g. 5 in the MHTGR-350 model) and in the 5<sup>th</sup> fuel block from the top (i.e. in the axial center of the core). Figure 6-11 shows that the axial-power profiles of the temperature-coupled OECD/NEA MHTGR-350 and isothermal IAEA CRP models differ substantially. Because there is no temperature feedback for the Phase II cases, and all fuel blocks are identical, the power profile for the unrodded CRP core is almost cosine. In contrast, the MHTGR-350 model has a 400 K temperature increase over the core height, with the cold inlet at the top of the core, in addition to varying isotopics for each block, which together produced a much more top-peaked axial-power profile (the dotted line in Figure 6-11).

**Power Peaking:** The rodded cores also resulted in the highest mean PP values (Figure 6-12) due to the more peaked nature of the axial-power profiles when the rods are inserted. However, the differences in PPs are less than for the AO data. The PP standard deviations for the depleted core 2b-r are significantly higher than the fresh-core models, but still less than 0.16% (see Figure 6-12). The cross-section uncertainties, therefore, did not result in significant changes in the PP values for these models.

### ***Integral Parameter Uncertainties: Temperature Feedback Coefficients and Control-Rod Worth***

In addition to the eigenvalue and power data, mean and variances values for two other commonly used parameters can be extracted from these data sets. Isothermal-temperature reactivity-feedback coefficients can, for example, be calculated using identical core models at different temperatures. The temperature branch cases are required for the coupled calculation with feedback defined for Phase III (Chapter 5). The feedback coefficients can be calculated by comparing the two data sets at various temperatures (e.g. 900–1,200 and 1,200–1,600 K) as shown in Table 6-2 for the 2a-rR core. The coefficients over these two temperature ranges vary between  $-7.2 \pm 0.2$  pcm/K and  $-9.4 \pm 0.5$  pcm/K. The relative isothermal-temperature reactivity-feedback coefficient standard deviations vary between 2.8–5.6%. The uncertainties in cross-sections, therefore, lead to non-negligible uncertainties in the feedback coefficients, which influence the fuel temperatures during reactivity-feedback transients and should be considered during the fuel- and core-design processes.

By subtracting the rodded and unrodded cases, operational control-rod-worth values can also be calculated. The operational rod worth is defined as the worth of the rods when fully withdrawn from the nominal operating position, which is defined as the bottom of the first fuel block (e.g. 79 cm inserted). The control-rod worth standard deviations shown in Table 6-3 for the 2a-r, 2a-2b-r, and 2a-2b-l-r cores are small, but still of interest in control and shutdown-margin characterization (0.12–0.17%).

It should be noted that the mean rod-worth values are extremely low (e.g. less than 0.1%, or 100 pcm), compared to the usual range for HTGR designs (i.e., 800–2,000 pcm, depending on load-follow requirements [Tyobeka, et al., 2007]).

It was shown in Figure 6-11 that power is much less peaked at the top of these isothermal cores compared to the OECD/NEA MHTGR-350 model, where the rods are worth ~850 pcm. The standard deviations on these small numbers could, therefore, not be a realistic representation of these uncertainties for the core with temperature feedback. This aspect is assessed again in Chapter 6 for the coupled core case Ex. III-1, where larger rod worths and uncertainties can be expected because the rods are located at the axial-power peak.

Table 6-2. Isothermal temperature-feedback coefficients (pcm/K) for core-2a-rR.

| Sample metric  | 1600K to 1200K | 1200K to 900K |
|----------------|----------------|---------------|
| $\mu$          | -7.23          | -9.42         |
| $\sigma$ (abs) | 0.20           | 0.52          |
| $\sigma$ (%)   | -2.80          | -5.57         |

Table 6-3. Control-rod-worth mean and standard deviations (%) for 1,000 samples of the fresh (2a) and mixed (2a-2b, 2a-2b-l) cores at 1,200K.

|              | 2a-r   | 2a-2b-r | 2a-2b-l-r |
|--------------|--------|---------|-----------|
| $\mu$ (%)    | -0.059 | -0.091  | -0.091    |
| $\sigma$ (%) | 0.146  | -0.165  | -0.117    |

Table 6-4. Effect of using Supercell I for three cores.

| Core         | 2a      | 2a-2b   | 2a-2b-R |
|--------------|---------|---------|---------|
| $k_{eff}$    |         |         |         |
| $\mu$        | -0.0114 | -0.0061 | -0.0061 |
| $\sigma$ (%) | -0.0012 | -0.0008 | -0.0006 |
| AO           |         |         |         |
| $\mu$        | 0.00001 | -0.0002 | 0.0005  |
| $\sigma$ (%) | -0.2597 | 0.7691  | 0.6436  |
| PP           |         |         |         |
| $\mu$        | -0.0103 | -0.0084 | -0.0088 |
| $\sigma$ (%) | 0.0073  | 0.0063  | 0.0093  |

### ***The Effect of Supercell L on Uncertainties***

One objective of this study was to assess the effect uncertainties of a better representation of the spectral environment at the core periphery during the generation of fuel cross-sections on the FOM. The benefit of using supercells to improve nominal local reaction rates has been demonstrated for HTGRs (Ortensi 2012), but their impact on HTGR uncertainties has not yet been quantified.

Table 6-4 shows the difference between the mean and standard deviations for three core models when cross-sections from Supercell *l* are used at the core periphery. The values are presented here as the differences between the  $k_{\text{eff}}$ , AO, and PP data sets. For example, for the first and last columns of the table, the differences are defined as  $(\text{core-2a-l})_{\mu} - (\text{core-2a-r})_{\mu}$  and  $(\text{core-2a-2b-rR})_{\sigma} - (\text{core-2a-2b-l-rR})_{\sigma}$ . The impact of Supercell *l* on the mean  $k_{\text{eff}}$  values is significant: approximately 600 pcm (0.58%) for the mixed cores and up to 1144 pcm (1.07%) for the fresh core (2a-r). In all three cases, the use of Cell *l* led to lower eigenvalues. The same trend is observed for AO and PP data. This confirms the importance of using a softer spectral environment in these peripheral regions for nominal best-estimate calculations.

The effect on the  $k_{\text{eff}}$  standard deviations of these sample sets are, however, insignificant where the differences between the core models with and without Supercell *l* cross-section are less than 0.0025%. The AO and PP data sets show varying and somewhat larger impacts (from 0.009 up to 0.76%). These are very small variances, which suggests that the uncertainty in these integral FOMs are relatively insensitive to the spectral environment. The use of supercells *for uncertainty studies* is therefore not strictly necessary, but because their use does improve nominal results, it is nevertheless recommended.

The single rod example included here (i.e. core-2a-2b-rR) does not show a significant difference with the trends identified for the unrodded cores (i.e. the presence of control rods does not change the conclusions reached). For all these cases, a more-detailed study should, however, involve an assessment of local reaction rates (e.g. fluxes, power levels) to confirm these integral trends.

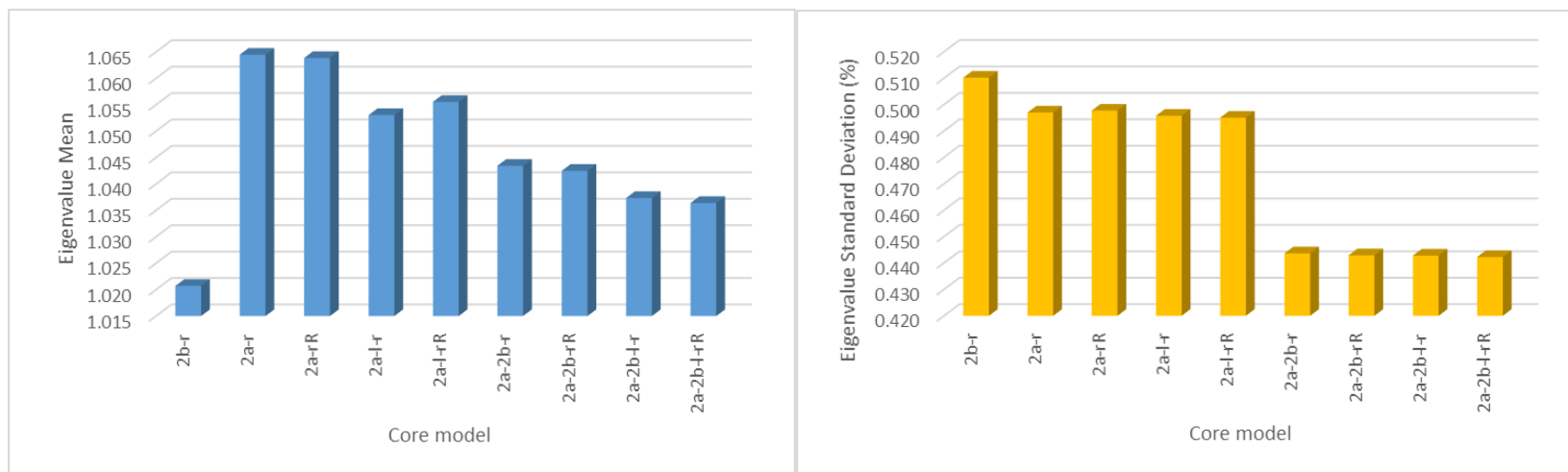


Figure 6-9.  $k_{eff}$  comparison of 26-group  $\mu$  (left) and  $\sigma$  (%) (right) for eight P/R core models.

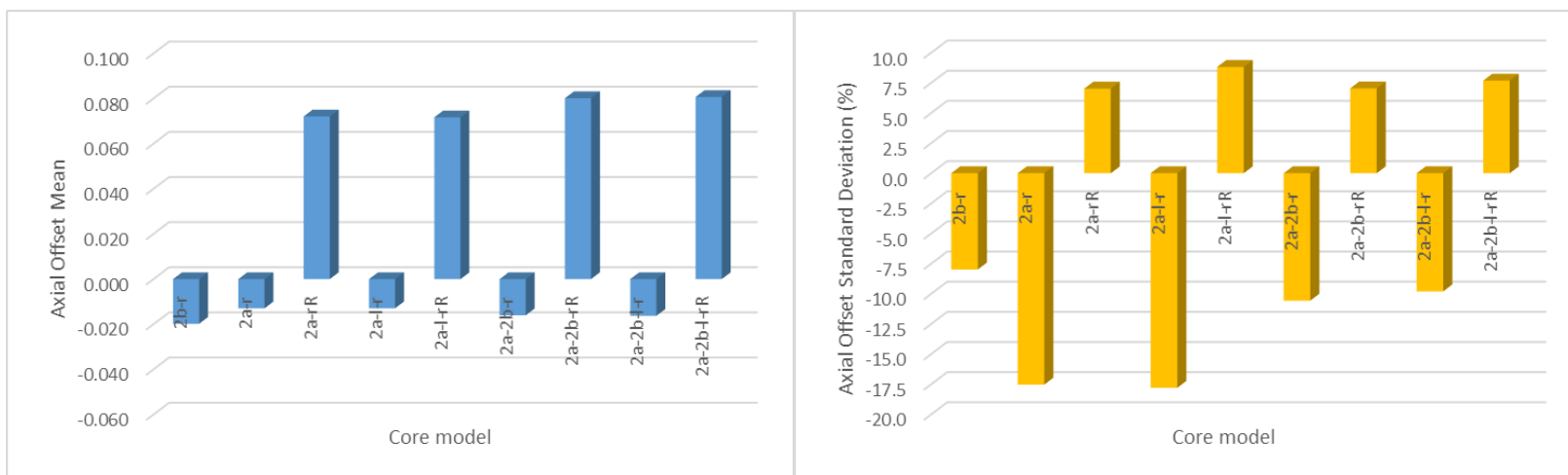


Figure 6-10. AO comparison of 26-group  $\mu$  (left) and  $\sigma$  (%) (right) for eight P/R core models.

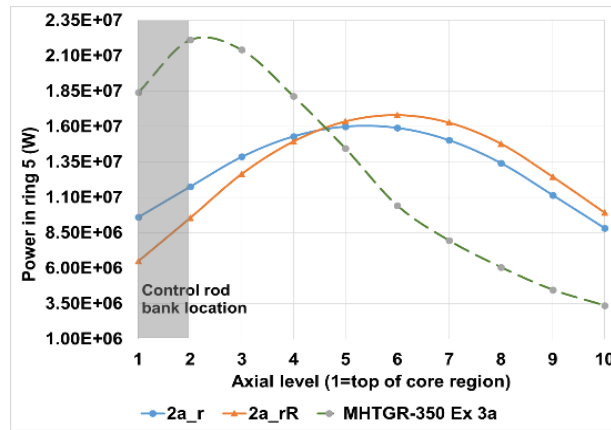


Figure 6-11. Comparison of Ring 5 axial power (W) distributions for the rodded (2a-rR) and unrodded (2a-r) fresh core vs. MHTGR-350 benchmark model with thermal feedback.

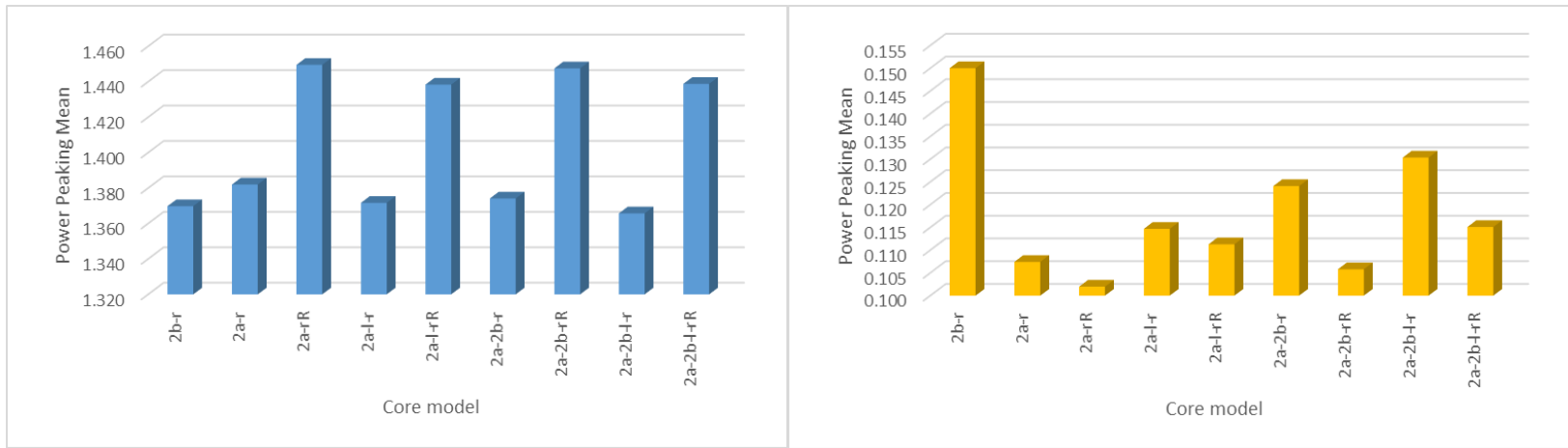


Figure 6-12. PP comparison of 26-group  $\mu$  (left) and  $\sigma$  (%) (right) for eight P/R core models.

### Uncertainties in Spatial Power Data

Integral parameters like the core eigenvalue or  $\lambda$  are useful indicators of trends during the initial comparison phase, but the impact of cross-section uncertainties also needs to be assessed for local reaction rates, fluxes, and power densities. As an example of these spatial distributions, the power profile in Fuel Rings 3 (inner), 4 (center), and 5 (outer) is shown in Table 6-5 for the core-2a-r model. Axial Level 1 is at the top of the core. The table presents the mean power distribution in absolute and relative units in the three rings for the 1,000 P/R Core 2a-r cases. A subset of this data is shown in Figure 6-13 for Rings 3 and 5. The peak power generation is in the outer fuel ring next to the reflector and in the axial center of the core, where almost double the power per mesh is produced compared to the top and bottom areas of the core.

The power mean and standard deviations for all eight core models are compared in Table 6-6. For clarity, only the mean and standard deviations of the power generated in Ring 5 are included here. The standard deviation in the local power ranges from 0.11–1.52%, which is significantly larger in some regions than the impact the cross-sections had on the core eigenvalue. The standard deviation varies inversely with the absolute power profile; the highest deviations occur in the top and bottom regions of the core, where the least power is generated (Figure 6-14). The inverse correlation is especially pronounced for the rodged models, where the power profile is shifted downwards. As discussed in Section 6.2.3, the regions with the highest deviations occur next to the upper, lower and side reflectors, where the reflector region changed the spectrum that the fuel region experiences and, therefore, the relative sensitivities of some cross-section covariances. It is interesting to note how similar the power profiles are for these core models, ranging from fresh (2a-r) to fully depleted (2b-r) and mixed loading patterns, especially in the higher power production regions.

Table 6-5. Core-2a-r power distribution mean.

| Axial level | Sample mean power (MW) |        |        | Mean power (% of 350 MW) |        |        |
|-------------|------------------------|--------|--------|--------------------------|--------|--------|
|             | Ring 3                 | Ring 4 | Ring 5 | Ring 3                   | Ring 4 | Ring 5 |
| 1 (top)     | 8.19                   | 8.01   | 9.45   | 2.34                     | 2.29   | 2.70   |
| 2           | 9.96                   | 9.42   | 11.68  | 2.85                     | 2.69   | 3.34   |
| 3           | 11.82                  | 11.17  | 13.88  | 3.38                     | 3.19   | 3.97   |
| 4           | 13.10                  | 12.38  | 15.39  | 3.74                     | 3.54   | 4.40   |
| 5           | 13.72                  | 12.98  | 16.12  | 3.92                     | 3.71   | 4.61   |
| 6           | 13.66                  | 12.92  | 16.05  | 3.90                     | 3.69   | 4.59   |
| 7           | 12.92                  | 12.21  | 15.18  | 3.69                     | 3.49   | 4.34   |
| 8           | 11.53                  | 10.90  | 13.54  | 3.29                     | 3.11   | 3.87   |
| 9           | 9.57                   | 9.04   | 11.22  | 2.73                     | 2.58   | 3.21   |
| 10          | 7.67                   | 7.50   | 8.85   | 2.19                     | 2.14   | 2.53   |

Table 6-6. Mean power (MW) and standard deviation (%) profiles in ring 5 for eight core models.

| Axial Level            | 2b-r  | 2a-r  | 2a-rR | 2a-l-r | 2a-2b-r | 2a-2b-rR | 2a-2b-l-r | 2a-2b-l-rR |
|------------------------|-------|-------|-------|--------|---------|----------|-----------|------------|
| 1                      | 10.86 | 9.45  | 9.42  | 9.42   | 10.08   | 6.73     | 10.06     | 6.71       |
| 2                      | 12.43 | 11.68 | 11.61 | 11.61  | 12.00   | 9.66     | 11.95     | 9.60       |
| 3                      | 14.22 | 13.88 | 13.79 | 13.79  | 14.01   | 12.73    | 13.94     | 12.65      |
| 4                      | 15.42 | 15.39 | 15.28 | 15.28  | 15.38   | 15.00    | 15.29     | 14.90      |
| 5                      | 15.98 | 16.12 | 16.00 | 16.00  | 16.03   | 16.40    | 15.93     | 16.30      |
| 6                      | 15.87 | 16.05 | 15.93 | 15.93  | 15.94   | 16.89    | 15.84     | 16.79      |
| 7                      | 15.09 | 15.18 | 15.07 | 15.07  | 15.11   | 16.43    | 15.02     | 16.33      |
| 8                      | 13.68 | 13.54 | 13.45 | 13.45  | 13.58   | 15.04    | 13.51     | 14.97      |
| 9                      | 11.71 | 11.22 | 11.16 | 11.16  | 11.43   | 12.83    | 11.37     | 12.78      |
| 10                     | 9.90  | 8.85  | 8.82  | 8.82   | 9.32    | 10.54    | 9.29      | 10.53      |
| Standard Deviation (%) |       |       |       |        |         |          |           |            |
| 1                      | 1.27  | 1.16  | 1.12  | 1.16   | 1.21    | 1.29     | 1.21      | 1.35       |
| 2                      | 0.62  | 0.59  | 0.83  | 0.59   | 0.58    | 0.96     | 0.58      | 1.03       |
| 3                      | 0.28  | 0.31  | 0.64  | 0.31   | 0.27    | 0.72     | 0.27      | 0.79       |
| 4                      | 0.12  | 0.16  | 0.42  | 0.16   | 0.12    | 0.48     | 0.12      | 0.52       |
| 5                      | 0.15  | 0.11  | 0.20  | 0.11   | 0.12    | 0.22     | 0.13      | 0.24       |
| 6                      | 0.18  | 0.13  | 0.10  | 0.14   | 0.15    | 0.11     | 0.16      | 0.12       |
| 7                      | 0.16  | 0.19  | 0.34  | 0.20   | 0.15    | 0.36     | 0.15      | 0.40       |
| 8                      | 0.12  | 0.27  | 0.60  | 0.28   | 0.18    | 0.64     | 0.16      | 0.70       |
| 9                      | 0.29  | 0.44  | 0.90  | 0.45   | 0.34    | 0.95     | 0.32      | 1.04       |
| 10                     | 0.78  | 0.86  | 1.37  | 0.88   | 0.80    | 1.41     | 0.79      | 1.52       |

### Comparison between 26-Group and 8-Group Results

The objective of this section is to assess the impact of few-group structure on the mean and standard-deviation values obtained for the various core models. Due to space limitations, only the results from the SCALE 8-group structure (see Table 2-4 in Chapter 2) are compared with the FZJ 26-g structure. The trends between these two sets of core models are discussed for  $k_{\text{eff}}$  only.

The contrast between the mean and standard deviation results obtained for the two group structures can be seen by comparing Figure 6-15. The 26-group mean eigenvalues are significantly higher than the 8-group values for all the core models, but the standard deviations are almost identical (i.e., less than 5 pcm). The eigenvalue differences are more clearly shown in Figure 6-16, where the burned core 2b-r had the largest difference (~900 pcm, or around 0.9%). The 8-group structure seems to be particularly sensitive to the addition of burned fuel to the core models, possibly caused by the choice of energy-group boundaries that were not optimized for the resolution of plutonium resonances. The mixed-core eigenvalues differ by a similar degree, but the fresh-core variants differ by less than 200 pcm.

For all best-estimate steady-states, and faster reactivity-feedback transients, a higher number of energy groups should be used. The 8-group structure can, however, still be useful for best-estimate assessments of transient cases where computational time is important (e.g. a re-critical loss-of-cooling event), especially during the conceptual core-design phase. In contrast to this recommendation, it is shown here that the 26- and 8-group eigenvalue standard-deviation results (0.44–0.51% for these eight core examples) are not sensitive *at all* to the group structures, and the additional expense of performing a large number of statistical perturbations using more than eight groups for U/SA purposes is not justified.

### **Summary of Ex. II-2a/2b Uncertainty Results**

A summary is provided in Table 6-7 of the impact of covariance uncertainties in the cross-section data on selected FOMs. The table lists the absolute standard deviations (in percentages) for the eight core-model data sets, each consisting of 1,000 P/R calculations performed at 1,200 K. Only the data calculated for the 26-group sample set are shown here because the 8-group uncertainty ranges are very similar.

The first column shows the range of the local power uncertainties varying from 0.10 to 1.52% for Ring 5. The variances between fresh and mixed/depleted core models are not as great as the axial variations between the top and bottom within each core model. In the context of general reactor-physics simulations, uncertainties in local power levels of more than 1% are usually seen as significant, which is the case in the upper and lower regions of the core.

The remaining four FOMs are integral indicators commonly used in core-design simulations. The core eigenvalue uncertainty ranges between 0.44 and 0.51%, which is large in comparison to the typical differences seen between nominal deterministic and Monte Carlo transport solutions (less than 0.1%). The PP and AO uncertainties are smaller (e.g. 0.10–0.15%) and are probably below the level of significance in typical core-design metrics.

The uncertainty range in control-rod worth (0.12–0.15%) is likewise small, but it has been noted that this result could be limited to the isothermal models used for these Phase II-2 benchmark cases. For the three data sets included in this chapter, an uncertainty on the rod worth of less than 0.15% is not significant. It is furthermore debatable whether the 2.80–5.57% variance calculated for the Core 2a-rR isothermal-feedback coefficients are important because this is mostly a function of fuel design that cannot be varied much for modern HTGRs.

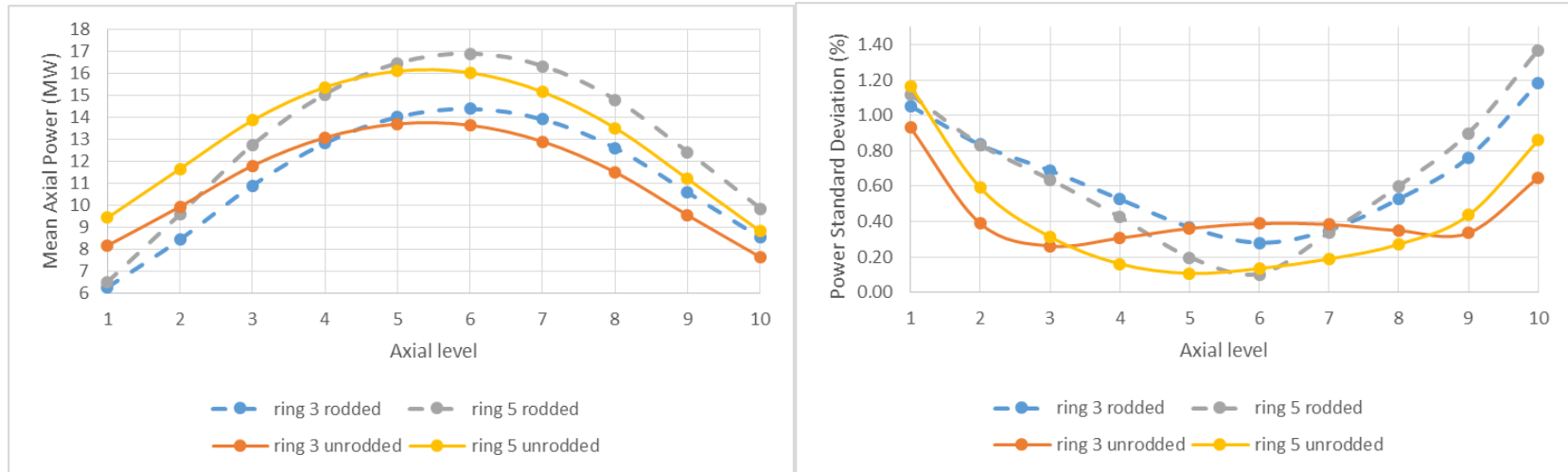


Figure 6-13. Mean axial power (MW) (left) and standard deviation (%) (right) profiles in Fuel Rings 3 and 5 for the rodded (2a-rR) and unrodded (2a-r) cores.

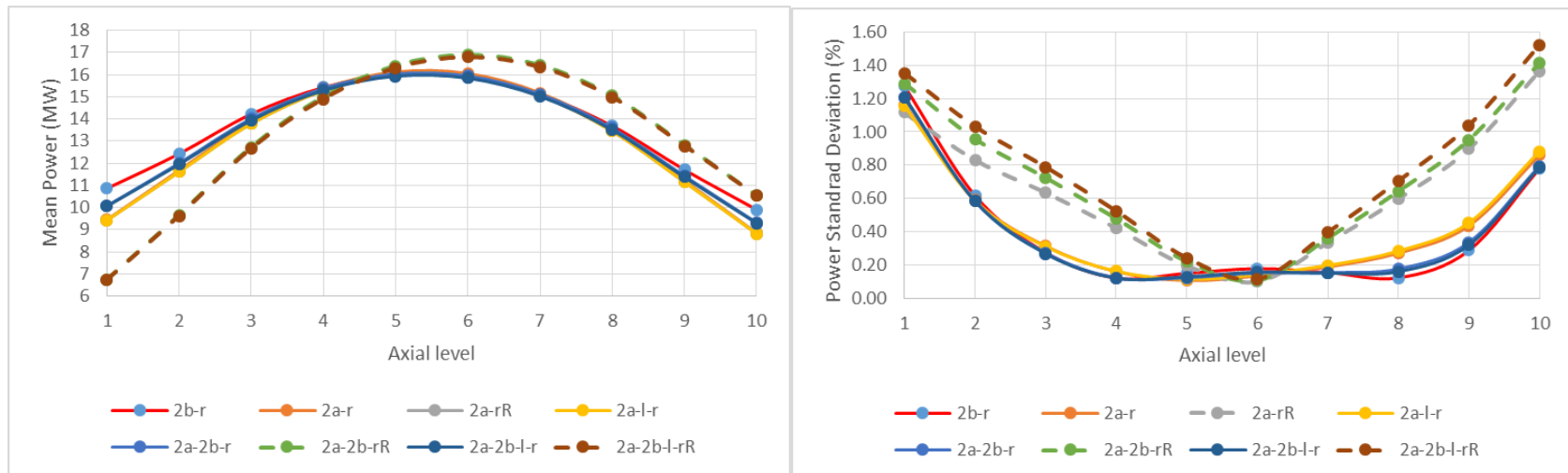


Figure 6-14. Mean axial power (MW) (left) and standard deviation (%) (right) profiles in Fuel Ring 5 for eight core models.

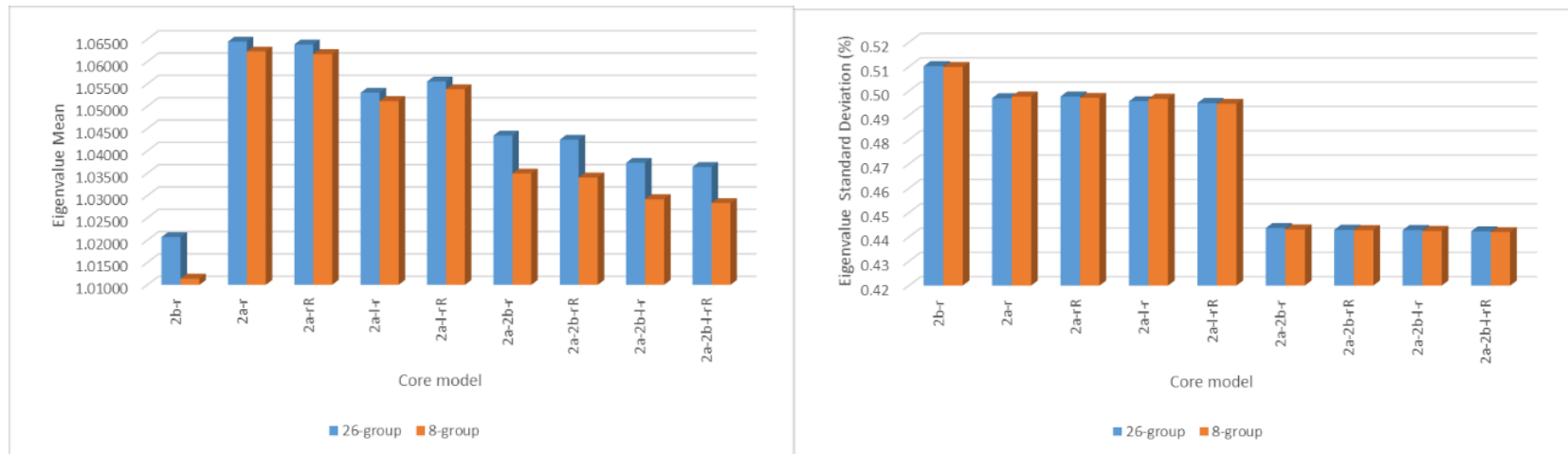


Figure 6-15. Eigenvalue comparison of 26- and 8- group  $\mu$  (left) and  $\sigma$  (%) (right) for eight P/R core models.

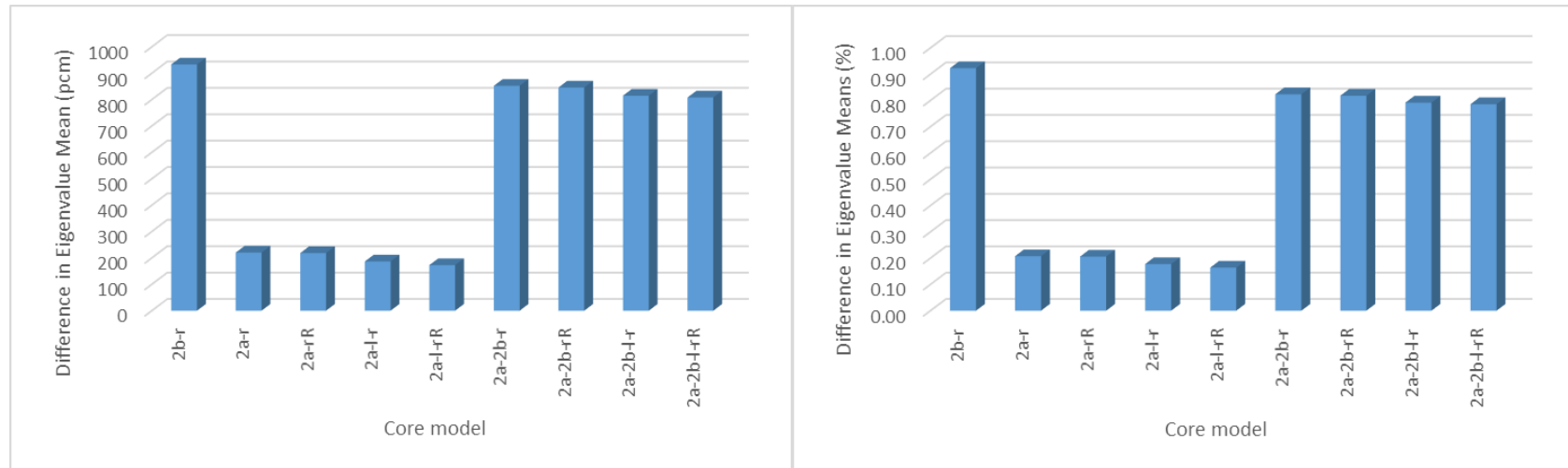


Figure 6-16. Absolute (left) and relative to the 26-g mean values (%) (right) difference between the 26- and 8-group eigenvalue means.

Table 6-7. P/R sample standard deviation (%) for eight core models (26-group data).

| Core Model | Sample Standard Deviation $\sigma$ (%) |                          |               |              |          |                                             |
|------------|----------------------------------------|--------------------------|---------------|--------------|----------|---------------------------------------------|
|            | Axially Averaged Power in Ring 5 (MW)  | Eigenvalue ( $k_{eff}$ ) | Power Peaking | Axial Offset | CR Worth | Isothermal Temperature-Feedback Coefficient |
| 2b-r       | 0.12–1.27                              | 0.51                     | 0.15          | 0.15         | -        | 2.80–5.57                                   |
| 2a-r       | 0.11–1.16                              | 0.50                     | 0.11          | 0.11         | 0.15     |                                             |
| 2a-rR      | 0.10–1.37                              | 0.50                     | 0.10          | 0.10         |          | 2.80–5.57                                   |
| 2a-l-r     | 0.11 -1.16                             | 0.50                     | 0.11          | 0.11         | -        |                                             |
| 2a-2b-r    | 0.12 -1.21                             | 0.44                     | 0.12          | 0.12         | 0.17     |                                             |
| 2a-2b-rR   | 0.11–1.41                              | 0.44                     | 0.11          | 0.11         |          |                                             |
| 2a-2b-l-r  | 0.12–1.21                              | 0.44                     | 0.13          | 0.13         | 0.12     |                                             |
| 2a-2b-l-rR | 0.12–1.52                              | 0.44                     | 0.12          | 0.12         |          |                                             |

### 6.2.3 Exercise II-2a and II-2b Sensitivity Results

In this section, a summary of the sensitivity data obtained with RAVEN is provided for the P/R Phase II neutronics stand-alone exercises. Due to space limitations, only a few examples of the available data set are included here (e.g. only eigenvalue trends), with the discussion of AO and PP results deferred to Section 8.1.3, where temperature feedbacks play an important role.

A summary comparison of the Phase I and II  $k_{eff}$  NSCs and PCCs are presented in Figure 6-17 and Figure 6-18, respectively. A few general observations can be made about trends observed for this data set:

- The direct equivalents of fresh and depleted lattice models I-2a and I-2b are Cores 2a-r and 2b-r, respectively. The only difference between these models are the softer spectrum caused by the addition of graphite reflectors (vs. the harder spectrum of infinitely reflected fuel blocks for the lattice models), and the change in energy-group structures (252-group NEWT vs. 26-group P/R). The PCCs and most of the sensitivity coefficients for these four models Figure 6-18 compare very well, with the same ranking calculated for both fresh and depleted geometries. As observed for the VHTRC and Phase I data, the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction ranks in the first place for all Phase II core models as well, followed by the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  reaction for the fresh cores. For the mixed cores, the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  reaction had the seconds highest ranking, with a consistent slight decrease in the NSCs observed between the cores containing mixed and depleted-only fuel.

- The addition of the control rods did not change the ranking order between Cores 2a-r and 2a-rR, but as noted before, both the NSCs and the degree of linear correlation (i.e. the PCC values) is higher for the rodded cores.

The addition of borated material in the reflector therefore enhanced the impact of the uncertainties in the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction, primarily due to the change in the core neutron spectrum.

- One of the objectives of this study was to identify the impact of the peripheral Cell *I* on sensitivity parameters. If the two sets of Ex. II-2a fresh and Ex. II-2b mixed-core coefficients are compared (i.e. 2a-r vs. 2a-l-r, and 2a-2b-rR vs. 2a-2b-l-rR), it is clear that neither the ranking nor the amplitudes of the PCCs and NSCs are affected significantly by the addition of Cell *I*. The only noticeable change is the increase in the NSC for the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction when the peripheral Cell *I* is included. Similar to the conclusion reached in Section 3.3.2 for the uncertainty impacts of Cell *I*, it is therefore also concluded here that the use of such a peripheral cell to represent spectral effects at the core boundaries is not important for eigenvalue-sensitivity parameters. As stated before, the worth of such a model representation for *best-estimate* calculations is not disputed, but it seems that for HTGR uncertainty and sensitivity assessments the simpler—and computationally less expensive—“basic” core models would be acceptable.

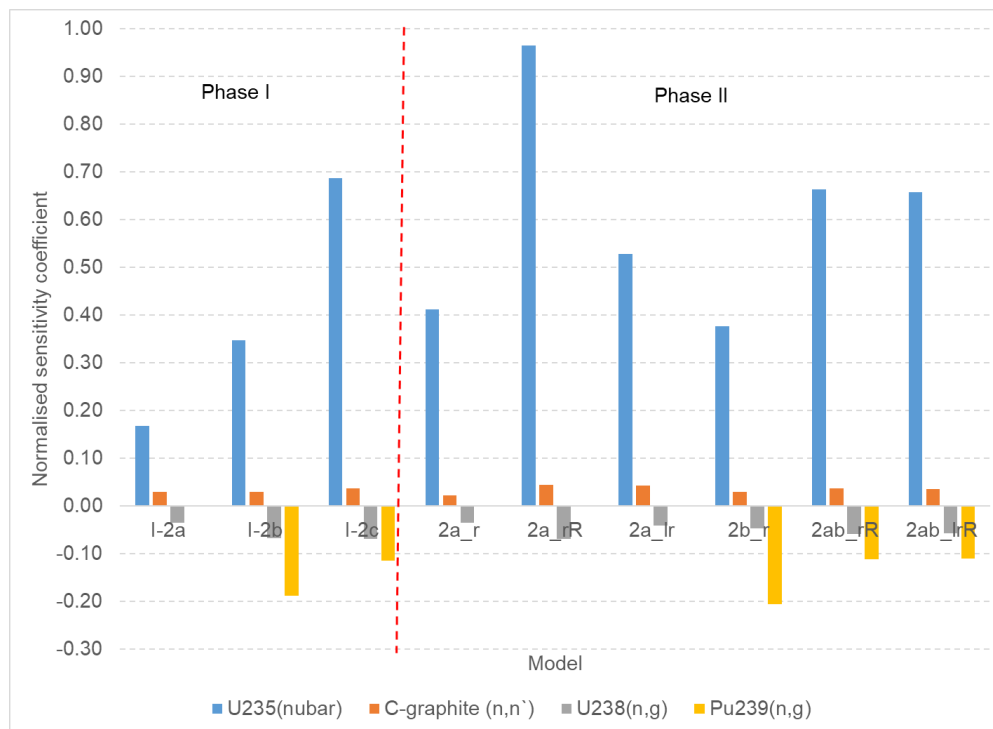


Figure 6-17. Comparison of Phase I and II  $k_{\text{eff}}$  NSCs for the  $^{235}\text{U}(\bar{\nu})$ , C-graphite elastic scatter,  $^{238}\text{U}(n,\gamma)$  and  $^{239}\text{Pu}(n,\gamma)$  reactions.

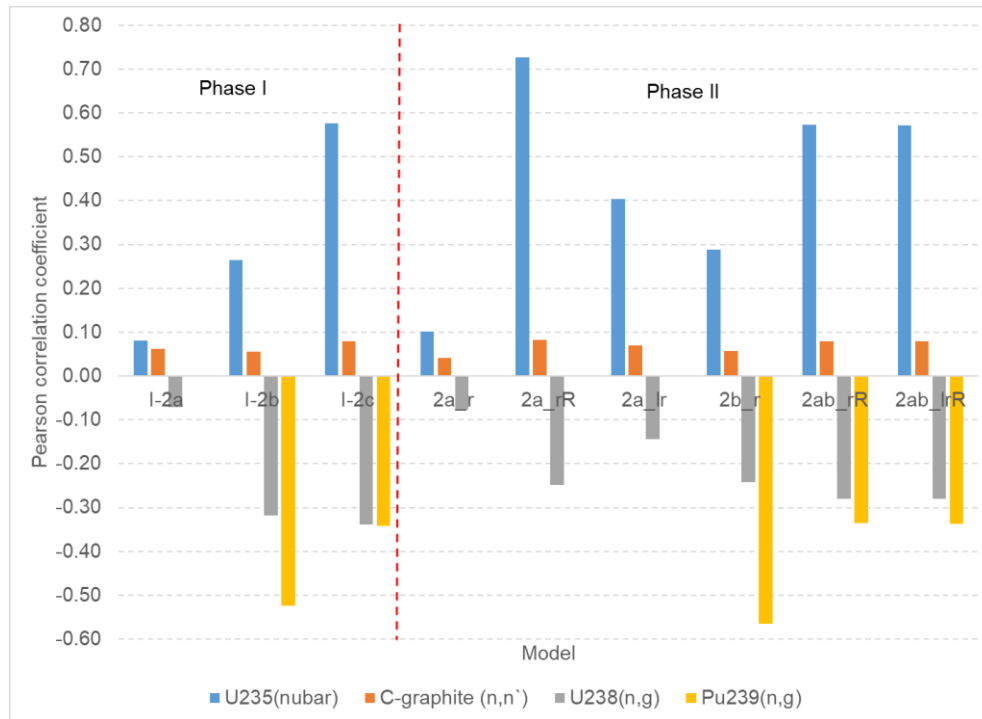


Figure 6-18. Comparison of Phases I and II  $k_{\text{eff}}$  PCCs for the  $^{235}\text{U}(\bar{\nu})$ , C-graphite elastic scatter,  $^{238}\text{U}(n,\gamma)$  and  $^{239}\text{Pu}(n,\gamma)$  reactions.

The  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  sensitivity and PCCs obtained for six of the core-model combinations are presented in Figure 6-19 for  $k_{\text{eff}}$  as a typical example of general trends. In general, Phase I and II sensitivity data are very similar; e.g. a comparison of Figure 5-11 for the three Phase I lattice cells with Figure 6-19 indicates the same smooth, uniform region below 1 eV and variances in the epithermal-resonance region. This can be expected because the 56-group covariance data are implicitly folded into the perturbed libraries used to construct core models. However, the addition of graphite in the reflector region changed the spectrum that the fuel region experiences and, therefore, the relative sensitivities of some cross-section covariances.

This can best be seen in the case of Core 2a-r, in which Phase II  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  sensitivity coefficients are mostly negative, compared to the small positive values observed for the corresponding lattice cell (2a) in Figure 5-11 in the same energy range. As already pointed out in the Phase I discussion, the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  PCCs for this case are very low and likely indicative of significant uncertainties in the sensitivity coefficient, so this result is not seen as significant. A more-direct illustration of the impact of the neutron spectrum on these parameters can be seen in Figure 6-19 from the addition of control rods (core 2a-rR) and Supercell I (Core 2a-l-r) to fresh Core 2a-r: in both these cases, the PCCs indicate significant linear correlations, and the sensitivity coefficients are likewise much larger than the unrodded Core 2a-r.

In the case of rodded Core 2a-rR, the additional absorption by the B<sub>4</sub>C in the control rods decreases (amongst other effects) the thermal backscatter by graphite into the core region, leading to a relative increase in the magnitudes of the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  thermal-region sensitivity coefficients. It can be seen in Figure 6-20 that the Mixed-Core 2a-2b-l-r produced significantly lower values for both  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  PCC and sensitivity-coefficient indicators. This is mainly caused by the decreased  $^{239}\text{Pu}$  (and increased  $^{238}\text{U}$ ) content of this core because both these factors would tend to decrease the relative importance of the  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  reaction on the overall core eigenvalue.



Figure 6-19.  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  sensitivity coefficients (top) and PCCs (bottom) for various 2a, 2a-2b and 2a-2b-l core models.

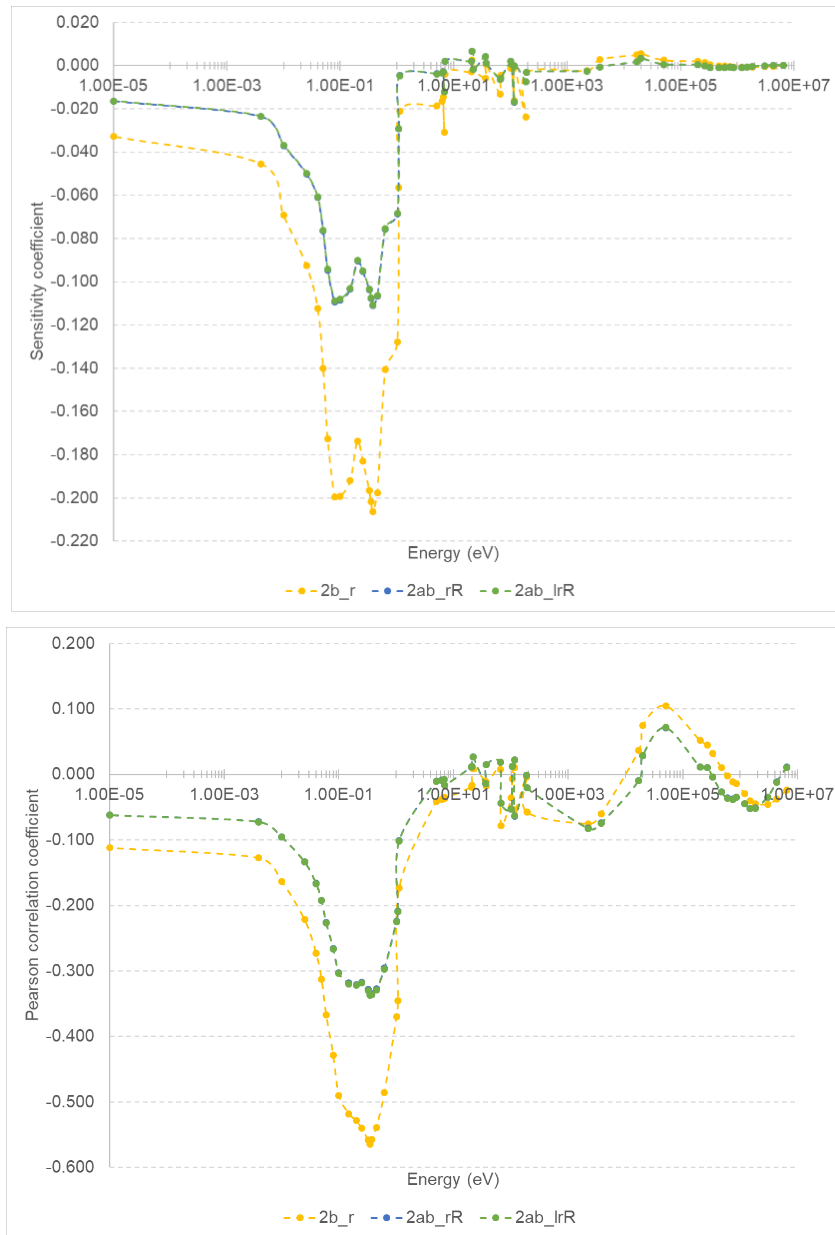


Figure 6-20.  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  sensitivity coefficients (left) and PCCs (right) for the 2b-r, 2a-2b-rR and 2a-2b-lrR core models.

### 6.3 Conclusion

The focus of this chapter was on the propagation of cross-section uncertainties from the Phase I lattice models to the stand-alone neutronics Phase II P/R core models using the perturbed cross-section libraries created with the NEWT/Sampler/RAVEN statistical U/SA sequence described in Chapter 2. RAVEN was applied to determine the uncertainty metrics and energy-dependent sensitivities and PCCs.

The main objectives were the assessment of the Phase II, Ex. II-2a and 2b stand-alone neutronics core-model uncertainty and sensitivities, and comparison with the Phase I Ex. I-2a, 2b, and 2c lattice results. For Phase II core models, it was shown (Table 6-1) that the core  $k_{\text{eff}}$  mean values vary up to 4% between the depleted (2b-r) and Ex. II-2a fresh core (2a-r), down to less than 0.6% for the Ex. II-2b mixed cores (2a-2b-r). In contrast to these large  $k_{\text{eff}}$  differences, the sample standard deviations only vary between 0.44 and 0.51%, which is a relatively tight uncertainty band for cores containing different fuel-loading patterns, rodged and unrodged reflector blocks and peripheral supercell cross-section libraries. It was therefore concluded that the  $k_{\text{eff}}$  uncertainties caused by cross-section data uncertainties are mostly insensitive to the spectral environment, but the two single-fuel type core variants (e.g. 2a-r, 2a-l-r and 2b-r) produced higher standard deviations than the mixed-core variants.

The uncertainties observed for the Phase II models were found to be very similar to the uncertainties calculated for the Phase I lattice models (0.50–0.54%), indicating that the propagation of the 252-group NEWT/Sampler cross-section covariance data into the 26-group P/R model preserved the implicit uncertainty information within the 1,000 perturbed core libraries.

One of the objectives of this study was to assess the effect on the FOM uncertainties of using a better representation of the spectral environment at the core periphery during the generation of fuel cross-sections. The benefit of using supercells to improve the nominal local reaction rates has been demonstrated for HTGRs (Ortensi 2012), but their impact on HTGR uncertainties has not yet been quantified. It was shown that the impact of using a peripheral Supercell *I* on the mean  $k_{\text{eff}}$  values is significant (0.58% for the mixed cores and up to 1.07% for the fresh-core 2a-r). This confirmed the importance of using a softer spectral environment in these peripheral regions for nominal best-estimate calculations. However, it was also found that effect on the  $k_{\text{eff}}$  standard deviations were insignificant, with differences between the core models with and without Supercell *I* cross-section lower than 0.0025%. The use of supercells *for uncertainty studies* is therefore not necessary, but since their use does improve nominal results, it is nevertheless recommended.

In general, Phase I and II sensitivity data were very similar since the 56-group covariance data is implicitly folded into the perturbed libraries used to construct the core models. As observed for the VHTRC and the Phase I lattice models, the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction ranks in the first place for all Phase II core models as well. Similar to the observations made for the impact on  $k_{\text{eff}}$  uncertainty, it was found that neither the ranking nor the amplitudes of the sensitivity indicators were affected by the addition of the core peripheral Cell 1. It therefore seems that for HTGR uncertainty and sensitivity assessments the simpler—and computationally less expensive—“basic” core models would be acceptable.

In summary, the application of the NEWT/Sampler/RAVEN sequence to the NEWT MHTGR-350 Phase I and P/R Phase II neutronics stand-alone models produced consistent findings in terms of the impacts of uncertainties in the cross-section data and the main sensitivity drivers. As the primary outcome, it was demonstrated that the statistical U/SA methodology can propagate the perturbed cross-section data as few-group libraries to the Phase II core models using the standard two-step core-physics approach (fine group lattice libraries collapsed as input to few-group core models), without requiring changes to the lattice and core-physics codes used.

## 7. MHTGR-350 EXERCISES II-4 AND IV-1: STAND-ALONE CORE THERMAL FLUIDS

*“Scientific knowledge is a body of statements of varying degrees of certainty - some most unsure, some nearly sure, but none absolutely certain.” Richard Feynman.*

The contributions of participants in the IAEA CRP on HTGR UAM benchmark have so far exclusively been focused on the impact of neutronic parameters, i.e. cross-sections (e.g. Sihlangu et al. 2019, Han et al. 2019, Grol et al. 2019, Hao et al. 2018) and material densities (Rouxelin 2019). In this section, the impact of thermal fluid uncertainties on the MHTGR-350 fuel temperature is discussed as one of the major contributions of this work to the CRP. The stand-alone core thermal fluid exercises are designed to isolate the impact of input uncertainties in thermal fluid boundary conditions and material properties, and do not include any feedback to the reactor neutronics; i.e. no updates to the core power distribution are made.

The discussion in this chapter covers two exercises defined for the HTGR UAM thermal fluids core Phase II (steady-state) and IV (transient). The definitions of Exercises II-4 and IV-1 are discussed in Section 7.1, and an overview of the MHTGR-350 thermal fluid input uncertainties (boundary conditions, material properties, bypass flows) and R/R uncertainty assessment methodology are provided in Section 7.2 and 7.3, respectively. This is followed by a discussion of the uncertainty and sensitivity results obtained for the RELAP5-3D MHTGR-350 steady-state Exercises II-4 in Section 7.4. The chapter is concluded in Section 7.5 with a discussion of the results obtained for the Exercise IV-1 PLOFC transient.

### 7.1 Specification of the IAEA CRP on HTGR UAM Stand-Alone Core Thermal-Fluid Cases

The draft IAEA CRP on HTGR UAM Phase II specification (Strydom 2018) defines Exercise II-4 as an HFP thermal fluid-only steady-state core simulation. The core power-density distribution is provided and fixed; i.e. there is no neutronics feedback. The objective of this exercise is the isolation of the effect of thermal fluid uncertainties on the maximum fuel temperature (MFT)<sup>36</sup> as primary FOM. A similar series of *best-estimate* cases were specified for the OECD/NEA MHTGR-350 benchmark Phase I as Exercises 2a-d, where the material thermophysical properties (e.g. conductivity, specific heat, and emissivity) were defined using either constant values or as complex correlations of temperature and fluence.

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<sup>36</sup> The RELAP5-3D model utilizes a representative fuel model described in Appendix B-1. The MFT is also defined in Section 6.2.1.

During the development of the Exercise II-4 UAM specifications, performed as an outcome of this dissertation, both of these approaches were investigated, and it was found that the uncertainty results were sufficiently similar to only report on the simpler material-property representation—i.e. the use of constant thermal conductivity and specific-heat values<sup>37</sup>.

A specific focus of this section is the impact of bypass-flow uncertainties on fuel temperature. Bypass flows have been shown to play an important role in the core and reflector heat distribution during DLOFC events (Strydom 2004, Johnson et al. 2009, Sun et al. 2011, Tak et al. 2013, Sun et al. 2018), but the author is not aware of an attempt to quantify the impact of bypass-flow uncertainties on operating fuel temperature.

For the OECD/NEA MHTGR-350 benchmark, the core-bypass flows were varied between 0 and 11% in seven reflector and in-core regions, as listed in Table 7-1 (Ortensi et al. 2018). The bypass flow is defined as the proportion of the inlet helium flow that does not flow through the coolant channels, and typically includes engineered bypass flows—e.g. in the inner and outer control-rod channels—and unintended leak flows in the gaps between neighbouring fuel and reflector blocks. The seven specified bypass flows are included in the RELAP5-3D model as ten one-dimension pipe-flow channels connected to the relevant heat structures, as indicated in brackets in Table 7-1. For the HTGR UAM, the same approach as the MHTGR-350 benchmark was taken, and the results obtained for two scenarios (0 and 11% bypass flow) are discussed in Section 7.4.1.

Table 7-1. Nominal bypass-flow distribution.

| Component                                                       | Nominal values<br>(% of total flow) |
|-----------------------------------------------------------------|-------------------------------------|
| In-core (FR1: BP_300, Fuel Ring 2: BP_400, Fuel Ring 3: BP_500) | 1.50                                |
| Inner reflector (BP_200, BP_210)                                | 0.50                                |
| Inner control-rod cooling (BP_230)                              | 1.20                                |
| Outer control-rod cooling (BP_600)                              | 1.80                                |
| Outer reflector (first ring) (BP_650)                           | 1.38                                |
| Outer reflector (second ring) (BP_700)                          | 1.62                                |
| Permanent side reflector (BP_121)                               | 3.00                                |
| Total                                                           | 11.00                               |

<sup>37</sup> The focus of this work is the relative uncertainties on nominal results, not the accuracy of the nominal results. The advantage of reporting on the perturbation of constant material property values is that other participants in the UAM can probably implement these variations easier in their models for comparison than the fluence- and temperature-dependent correlations specified in the MHTGR-350 benchmark Exercise I-2c and I-2d. A comparison of the nominal results obtained for Exercise 2 of the OECD/NEA MHTGR-350 benchmark can be found in the author's earlier publications (Strydom, 2013; Strydom, 2015).

## 7.2 Thermal-fluid Boundary Conditions and Material-Property Perturbations

The RELAP5-3D model utilized for the OECD/NEA MHTGR-350 Exercise I-2b was used as the basis of the steady-state calculation reported here—i.e. utilizing constant material properties and with seven defined bypass-flow channels<sup>38</sup>. The RELAP5-3D model is described in detail in the OECD/NEA MHTGR-350 benchmark INL report (Strydom et al. 2013) and journal paper (Strydom et al. 2015) and is briefly summarized in Appendix B-1 in this work.

The variations in the thermal fluid boundary and material-property correlations shown in Table 7-2 are specified in Table D-2 of the draft Phase II specifications (Strydom 2018), but some minor changes to these parameters were made during this work. It is assumed that the variations in all these parameters can be described by normal distributions, which is the same approach taken by the OECD/NEA LWR UAM team for Phase II-3 specifications of the LWR UAM (Hou 2019). The bounds of the normal distributions are assumed at three standard deviations, also in accordance with the guidance issued by the LWR UAM team.

Table 7-2. Exercise II-4 thermal fluid input parameters and one standard deviation (%) values

| Input Parameter                                                                       | Nominal value                                         | 1 $\sigma$ Uncertainty |
|---------------------------------------------------------------------------------------|-------------------------------------------------------|------------------------|
| <i>Boundary conditions</i>                                                            |                                                       |                        |
| Total reactor power                                                                   | 350 MW                                                | $\pm 1\%$              |
| Decay heat (PLOFC only)                                                               | Specified per block<br>(OECD/NEA MHTGR-350 benchmark) | $\pm 2.85\%$           |
| Core bypass                                                                           | 0% or 11%                                             | $\pm 1\%$              |
| Reactor inlet temperature                                                             | 259°C                                                 | $\pm 1\%$              |
| Helium mass-flow rate                                                                 | 157.1 kg/s                                            | $\pm 1\%$              |
| <i>Material properties</i>                                                            |                                                       |                        |
| Fuel graphite thermal conductivity                                                    | 20.0 W/m.K                                            | $\pm 7\%$              |
| Fuel graphite specific-heat capacity                                                  | 3.50E+06 J/kg.K                                       | $\pm 3\%$              |
| Reflector thermal conductivity<br>(replaceable H-451 / permanent reflectors H-2020)   | 37.0 W/m.K<br>35.0 W/m.K                              | $\pm 5\%$              |
| Reflector specific-heat capacity<br>(replaceable H-451 / permanent reflectors H-2020) | 3.50E+06 J/kg.K<br>3.13E+06 J/kg.K                    | $\pm 5\%$              |
| RPV thermal conductivity                                                              | 40.0 W/m.K                                            | $\pm 2.5\%$            |
| Core-barrel thermal conductivity                                                      | 17.8 W/m.K                                            | $\pm 2.5\%$            |

<sup>38</sup> The stand-alone RELAP5-3D model used here and the coupled P/R model in Chapters 6 and 7 are identical, apart from the use of a fixed power profile for the former and feedback via PHISICS spatial kinetics for the latter.

### 7.2.1 Boundary Conditions

Operational quantities like the reactor total power, inlet mass-flow rate and helium-gas temperature vary due to measurement uncertainties. These parameters are typically used as boundary conditions in reactor-simulation models and play an important role in uncertainty quantification. The boundary-condition uncertainties listed in Table 7-2 were obtained from a study commissioned by PBMR in 2004 (Strydom 2004), and were based on information obtained from the operation of the AVR and other German nuclear power plants. The same values were also used in a subsequent uncertainty study by the author to assess the impact of thermal fluid uncertainties on the peak fuel temperature (Strydom 2013).

As a cross-check, the boundary-condition values selected by the OECD/NEA LWR UAM benchmark team for the PWR, BWR and VVER reactor types are listed in Table 7-4 (Hou et al. 2019). The HTGR total power and helium mass-flow rate standard deviations are comparable to the PWR and BWR values, but the helium-gas temperatures are measured with larger uncertainties (up to 10 K) due to the difficulty of high-temperature thermocouple sensor positioning and long-term operational drift.

Table 7-3. Comparison of non-HTGR material-property perturbation values (Hou, et al. 2019)

| Parameter                   | BWR                             | PWR                                           | VVER                |
|-----------------------------|---------------------------------|-----------------------------------------------|---------------------|
| Coolant flow rate (%)       | $\pm 1.0$                       | $\pm 1.5$                                     | $\pm 4.5$           |
| Power (%)                   | $\pm 1.5$                       | $\pm 1.0$                                     | $\pm 0.3$           |
| Inlet fluid temperature (K) | $\pm 1.5$                       | $\pm 1.0$                                     | $\pm 2.0$           |
| Fuel thermal conductivity   | Normal, $\pm 5\%$ <sup>39</sup> | Normal, $\pm 5\%$<br>$\pm 10\%$ <sup>40</sup> | Normal, $\pm 5\%$   |
| Fuel specific heat          | Normal, $\pm 1.5\%$             | Normal, $\pm 1.5\%$                           | Normal, $\pm 1.5\%$ |

Decay-heat uncertainty is based on the Deutsches Institut für Normung e.V. (DIN) standard (German National Standard 1990) for pebble-bed HTGRs because no other dedicated estimate of HTGR decay-heat uncertainties currently exists. Sampler can possibly be used to assess uncertainties in the decay heat production of the relevant isotopes, since the covariance data also include estimates of decay heat uncertainties. Alfonsi et al (2018) also used RAVEN to construct a reduced order model of HTGR decay heat models that allow many perturbed SCALE/ORIGEN parameters to be considered. The DIN standard recommends a standard deviation value of 2.85%, based on the derivation of the decay-heat correlation factors. The nominal decay-heat values are specified in the MHTGR-350 benchmark for each fuel block.

<sup>39</sup> LWR UAM Exercise II-1 specifications

<sup>40</sup> LWR UAM Exercise I-7 specifications

This parameter is not perturbed for the steady-state Exercise II-4, but it is varied as input to the Exercise IV-1 PLOFC transient discussed in Section 7.5.

### 7.2.2 Material Properties

The material-property uncertainties listed in Table 7-2 were also obtained from the 2004 PBMR study (Strydom 2004), and were based on information provided by the PBMR graphite and fuel suppliers. It was reported in the 2004 Time-dependent Neutronics and Temperatures (TINTE) study that the emissivity of the core barrel, reactor vessel, and reflector graphite influenced only local component temperatures and that uncertainties in the helium thermal physical properties did not result in significant changes to the MFT. These parameters were therefore not included in the assessment discussed here.

The specific-heat capacity<sup>41</sup> appears in the RELAP5-3D input as density  $\times$  specific heat; e.g. for H-451 at 1,000 K, it is  $1,850 \text{ kg/m}^3 \times 1,890 \text{ J/kg.K} = 3.50\text{E}+06 \text{ J/m}^3\text{.K}$ . By perturbing this parameter in RELAP5-3D with  $\sigma \pm 5\%$ , it can therefore be seen as either accounting for a 5% variation in the density of graphite or the specific heat of this material.<sup>42</sup>

### 7.2.3 Simulation of Core-Bypass Flow Variations

The behaviour of nuclear-grade graphite under irradiation, elevated temperatures, and stress loads is an active and complex field of materials research in the HTGR community. In general, all nuclear-graphite grades exhibit directional dimensional changes as a function of temperature, but since each graphite grade is manufactured using unique raw and binder materials, experimental data are required for each specific nuclear-graphite grade. The dimensional change, dimensional-change rate and coefficient of thermal expansion as a function of fast-neutron fluence is shown in Figure 7-1 (Marsden et al. 2016). Reactor-grade graphite typically shrinks during the first few years of exposure to high-energy neutrons and reaches a turnaround point after about 4–6 years before it starts swelling.

A systematic study of the change in bypass-flow fraction at various stages of prismatic-core life was reported by Kim and Lim (2011) using a detailed GAMMA+ model of the GT-MHR design. They found that the bypass-flow fraction can vary between 4.8 and 35% of the total inlet flow, leading to increases in the MFT of almost 200°C. In their work, a uniform 2 mm gap between all blocks in the core resulted in a bypass-flow fraction of 12%, which is close the value assumed in the MHTGR-350 benchmark and for this study.

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<sup>41</sup> The value of 1,890 J/kg.K for H-451 can be found by selecting 1,000K as input to the correlation in Table A-IV-3 of the OECD/NEA MHTGR-350 benchmark specification (Ortensi, 2018).

<sup>42</sup> For the coupled calculations in Chapters 6 and 7 this density perturbation is only performed on the RELAP5-3D model, i.e. the same variation is not applied to the SCALE/NEWT neutronics input.

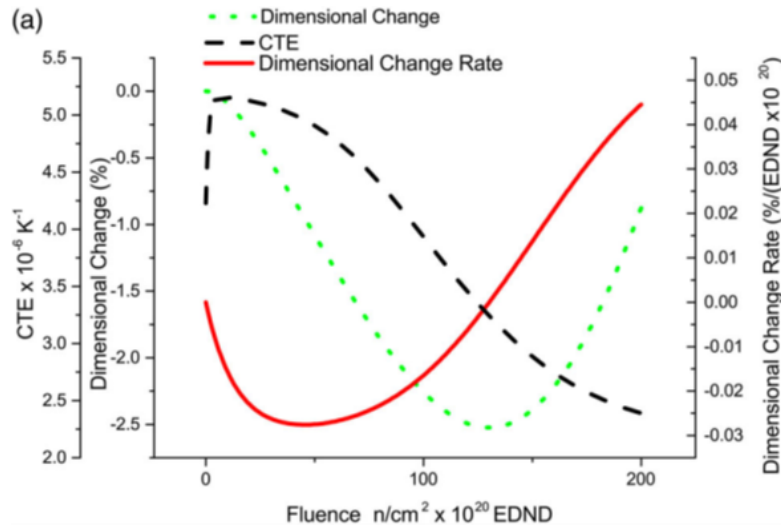


Figure 7-1. Typical dimensional and property changes in an isotropic graphite irradiated at  $\sim 500^\circ\text{C}$  (Marsden et al. 2016).

The author is not currently aware of any published full-core steady-state and LOFC uncertainty assessment of HTGR bypass flows. Drzewiecki (2013) performed a thermal fluid uncertainty assessment using the AGREE code and adjoint-based surrogate models of experimental data of the Helium Engineering Demonstration Loop experiment and the HTTR, but uncertainties in the bypass distributions did not seem to form part of the scope of his work. The approach described in this section is, therefore, a first attempt at quantifying the impact of bypass-flow uncertainties on the MFT and represents one of the author's contributions to the IAEA HTGR UAM.

Because bypass flow (and thermal conductivity) are both functions of fluence, several models at various “snapshots” over the core's lifetime need to be developed, representing the changes in both material properties and geometries. However, the spatial distribution of block-gap sizes can never fully be determined because that would require accurate tracking of all local-temperature and fluence histories for thousands of locations (the MHTGR-350 core contains more than 900 hexagonal fuel and reflector blocks with eight surfaces each). This parameter, thus, represents an epistemic input uncertainty in HTGR core simulation because it can (in principle) be reduced with high-fidelity computational fluid dynamics (CFD) models and enough computing power, but in practice, the bypass-flow uncertainty can never be reduced to zero. The problem is exacerbated by the use of simplified system-code models (e.g. TRACE, RELAP5-3D, Flownex) that typically assume some form of homogenization and only allow a limited representation of these intra-block leak flows.

In reactor safety studies, the steady-state (normal operation) problem can be bounded by taking the conservative approach for the highest fuel temperatures, which is the case when core-bypass flows are at their maxima (i.e. when gap sizes are at their largest) at the beginning of life. However, for the PLOFC transient, the situation is more complex: although the fuel temperatures generally decrease with less bypass flow, more bypass flow also leads to colder reflector and control-rod temperatures. Because the colder reflectors can absorb more energy during the PLOFC than the hotter reflector, a higher bypass-flow fraction usually leads to lower fuel temperatures during PLOFC, even if the starting point steady-state fuel temperatures are a little higher.

This principle is illustrated in Figure 7-2 and Figure 7-3 for the MHTGR-350 model. The sharp increase in the upper-region temperatures of the two reflector structures (Axial Levels 1–4) can be seen in Figure 7-2 for the steady-state case with bypass flow. It is also shown in Figure 7-3 that, although the PLOFC MFT with no bypass flows starts off 53 K lower than the case with no bypass flows (987 K vs.1040 K), the eventual PLOFC MFT peak is 88 K higher than the case with bypass flows. The rise in MFT also occurs significantly more slowly for the case with bypass flows due to the absorption of the core decay heat into the much colder reflector structures surrounding the core.

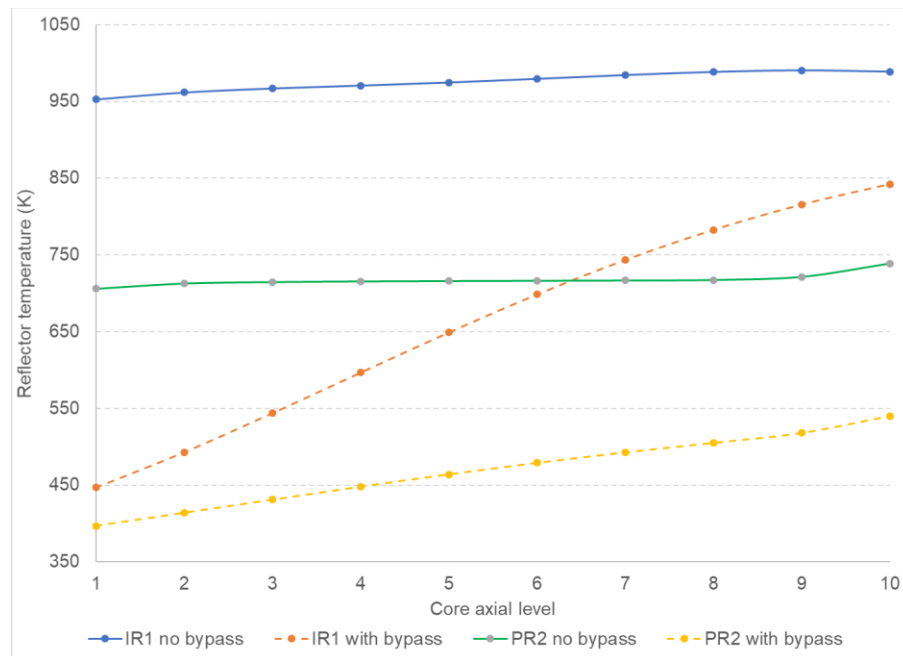


Figure 7-2. The impact of bypass flows on Inner Reflector Ring 1 (IR1) and Permanent Reflector Ring 2 (PR2) steady-state temperatures (Axial Level 1 = top of the core).

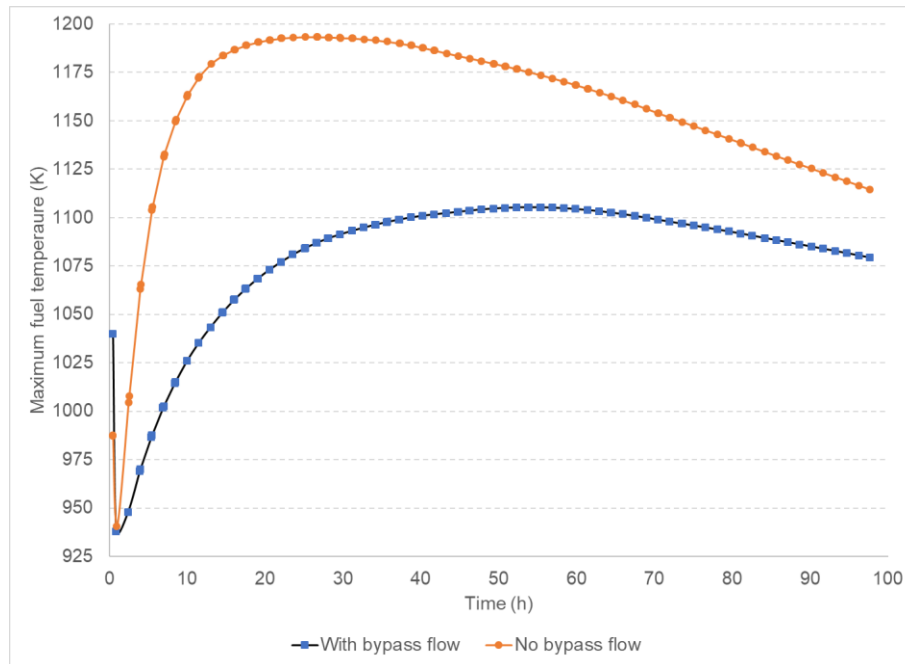


Figure 7-3. MFT as a function of time for the nominal MHTGR-350 models with and without bypass flows.

Two approaches are introduced in this work on the treatment of bypass flows in the RELAP5-3D model: a binary include/exclude assessment and the use of random sampling from a normal distribution defined for each of the seven defined bypass-flow channels. The first method involves the comparison of uncertainty and sensitivity parameters for two sets of simulations with the bypass flows included and excluded—i.e. assessing whether the inclusion of bypass flows in the model changes the MFT uncertainty or input-parameter sensitivity ranking.

The second method utilizes RAVEN to sample 1,000 perturbed values from normal distributions defined for each of the seven bypass-flow channels, as described in Section 7.3. A standard deviation of  $\pm 1\%$  is assumed for these sample distributions, with the limits defined at  $3\sigma$ , or  $\pm 3\%$ . The objective of this approach is to assess whether small perturbations in the reflector and core-flow distributions lead to significant changes in either the MFT uncertainty or the sensitivity ranking of the input parameters.

Because all flow channels in the RELAP5-3D model are connected to a common inlet- and outlet-plenum volume, a flow decrease in one channel will be redistributed to an increase in another flow channel. By perturbing all bypass flows simultaneously, the relative helium-flow distributions in the core model can therefore be influenced significantly.

In the sense that the MHTGR-350 model is based on end-of-life (EOL) data provided by GA (and the gap sizes are therefore fixed), this statistical perturbation representing randomized smaller and larger gap widths is somewhat artificial<sup>43</sup>, but it is nevertheless implemented to illustrate the possible contributions of the statistical-uncertainty methodology to the impact of this parameter.

As a final important remark, it should be indicated that consideration of the non-local heat disposition is not included in either of the OECD/NEA or IAEA HTGR UAM benchmark specifications because its consideration would require a high-fidelity gamma-transport solution of the MHTGR-350 EOL core state. As a result, because the non-local heat deposition in the reflector is approximately 6% of the total power (Strydom 2004), the current RELAP5-3D model will overestimate the impact of bypass-cooling flows, i.e. the reflector temperatures will be too low.

### 7.3 RAVEN/RELAP5-3D Thermal-Fluid Perturbation Methodology

The RAVEN/RELAP5-3D calculation sequence applied in this section is shown in Figure 7-4. As a first step, RAVEN is used to create 1,000 values for each of the input parameters listed in Table 7-2. The RAVEN/RELAP5-3D interface (Alfonsi et al. 2017) then subsequently creates 1,000 perturbed-input decks for RELAP5-3D and submits the cases to the computational cluster in parallel.

In contrast to the Sampler sequence, where the user is limited to 1,000 cross-section covariance samples, no limitations exist on the sample size of this sequence. It was however decided to keep the perturbed RELAP5-3D set matched with the 1,000 PHISICS cross-section libraries for the coupled Phase III and IV calculations (Chapters 6 and 7), even if individual RELAP5-3D steady-state core calculations were each completed within 30 minutes.

Narcisi et al. (2019) recently validated the RAVEN/RELAP5-3D sequence using experimental data from the NATural Circulation Experiment (NACIE) Facility, a non-nuclear loop-type system using lead-bismuth eutectic as coolant. However, as far as the author is aware, the work presented here is the first application of RAVEN on the thermal fluid behaviour of HTGR systems because the pioneering work of Rouxelin (2019) was limited the application of RAVEN to the neutronics aspects of prismatic HTGRs.

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<sup>43</sup> It should be noted that a more “biased” sampling approach was also considered, assuming that the gaps between high-fluence reflector blocks closer to the core were smaller than the gaps between the low-fluence blocks in the outer reflector region. However, because this model would depend on more-detailed knowledge of the ex-core flux distributions and the consideration of ex-core gamma and fast-neutronic heating, it was decided to bound the bypass-flow assessment by the “all-or-none” approach. More sophisticated and detailed studies can certainly be performed using computational fluid dynamics (CFD), or CFD-like, codes; the choice made here is commensurate with the approximate nature of the current “ring” homogenized RELAP5-3D model.

It is important to note that this sequence is artificial in the sense that changes in temperature distribution do not lead to changes in power distribution, which is the usual iterative scheme for core steady-state calculations.

Instead, the same power values are provided at each time step of the steady-state convergence process; i.e. in essence the power is “converged” from the first iteration while RELAP5-3D takes a few hundred-thousand iterations to converge all fluid flow and solid temperature fields. This “stand-alone” exercise was specifically designed for both the OECD/NEA MHTGR-350 and IAEA HTGR UAM benchmarks to study the effects of thermal fluid input parameters in isolation. The “standard” coupled neutronics and thermal fluids core calculation is discussed in Section 8.1 as a subset of Exercise III-1.

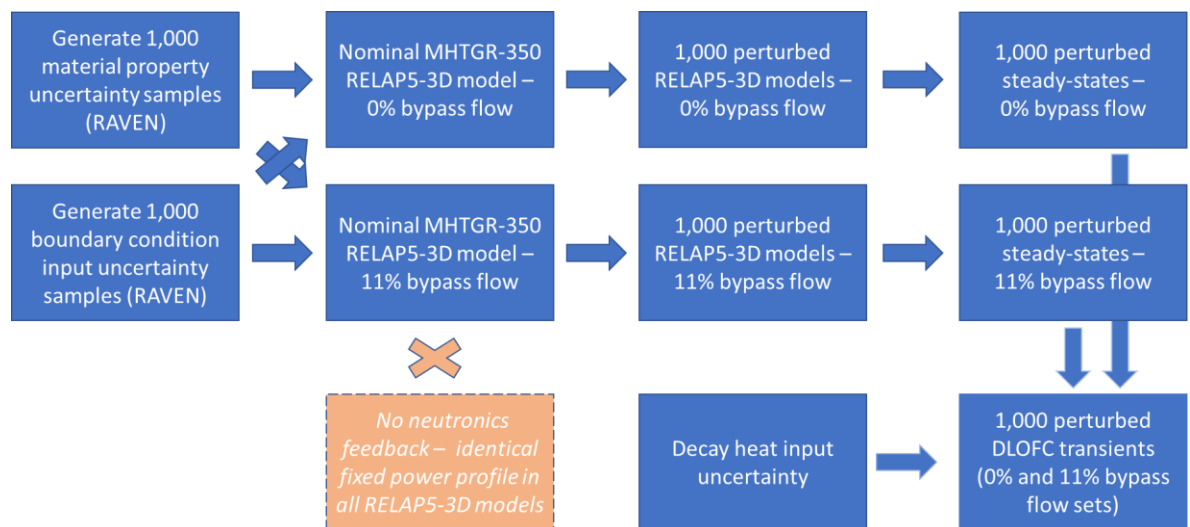


Figure 7-4. Calculation sequence for Exercises II-4 and IV-1.

The 0 and 11% bypass flow RELAP5-3D models are identical apart from the “restriction” of gas flow in the bypass-flow channels. This is achieved in RELAP5-3D by defining large values for the form-loss flow factor, defined on the xxx0900 input cards. This form-loss factor acts as a surrogate for throttled or restricted flow and is one of the user options to restrict the gas flow in a channel without removing the entire flow channel. In the case of the inner-reflector bypass flow, for example, the 7.85 kg/s helium flow in Pipe Element 210 is obtained by specifying a value of 50.0 on this card whereas practically zero flow (0.00085 kg/s) can be obtained by setting this value at 1,000,000, as shown below:

*With bypass:* 2100901 50.0 50.0 1

*Zero bypass:* 2100901 1000000.0 1000000.00 1

The remaining RELAP5-3D input parameters listed in Table 7-2 were modified in the following manner:

- **Total power, inlet mass-flow rate and gas temperature:** These three parameters occurs in only in four input cards in the RELAP5-3D deck, and the relevant cards were all modified with the same values simultaneously. As an example, for the first perturbed value of the total core power, RAVEN produced 355.63 MW. This value was replaced in the MHTGR-350 deck by the RAVEN interface parser in cards 30000001 and 20520000, which control the steady-state power set point and kinetics normalization, respectively, as shown in bold font below:

20520000 sspowfis constant **355637503.112**

30000001 no-gamma **355637503.112** 0.0 1.0 1.0 1.0

**Conductivity and specific heat capacity:** For the constant material-properties option, the thermal conductivity and specific-heat capacity of all materials in the RELAP5-3D model are specified in the xxx101 and xxx151 cards—e.g. as shown below for the thermal conductivity of graphite material #1.

\*MATERIAL NR 1 H-451 fluence 0

20100100 tbl/fctn 1 1

20100101 **66.0**

20100151 **3500000.0**

The RAVEN interface allows the user to target these cards directly and modify the tabulated values directly, according to the sampled distribution point.

- **Decay heat:** MHTGR-350 decay-heat data are based on ORIGEN calculations performed by the GA design team in the 1980s and provides the time-dependent decay heat up to 150 hours after shutdown. The OECD/NEA MHTGR-350 benchmark specification provides individual decay-heat (power) information for each of the 220 fuel blocks (Ortensi 2018). In the RELAP5-3D “ring” model, the fission and decay power generation are simplified to a single homogenized value per axial layer for each of the three fuel rings—i.e. 30 decay-heat entries in total. The decay-heat and fission-power summations are obtained through control variables defined in the input deck. These control variables can be modified directly by RAVEN based on the sampled value of the decay heat. In the example input-file entry below, the fission power and decay heat of the fuel blocks on Axial Level 7, Fuel Ring 3 is given by the control variables 2258 and 2267, respectively. The modified multiplicative decay-heat factor is inserted in the place of the 1.0 on card 20522682.

sum fission power and decay heat

20522680 CV2268 sum 1.0 0.0 1

20522681 0.0 1.0 cntrlvar 2258

20522682 **1.0** cntrlvar 2267

## 7.4 Exercise II-4: Thermal Fluids Stand-Alone Steady-State

### 7.4.1 Exercise II-4 Uncertainty Results

All steady-states were calculated for a total of 7,000 seconds to allow the thermal fluid and solid temperature fields to converge fully, but as indicated earlier, the core power distribution remained identical for each of the iterations. An example scatter plot of the RAVEN-generated total reactor-power input set is shown in Figure 7-5. These scatter plots can be used as confirmation that the sampling routine produced input parameters within the intended domain, e.g. in this case, that no values below 339.5 MW or above 360.5 MW (equal to  $3\sigma$ ) were selected. The scatter plot of the fuel temperature at axial level 10 in FR1 in Figure 7-6 likewise provides an indication of the range in the FOM ( $\sim 65$  K). The mean (1024 K) and standard deviation (9.5 K) values calculated from the 1,000 fuel-temperature samples for this core location are also shown in Figure 7-6. The full spatial data for all 30 fuel-temperature sets and the two model variants are presented in Table 7-4. The highest of these 30 fuel temperatures are designated as the MFT.

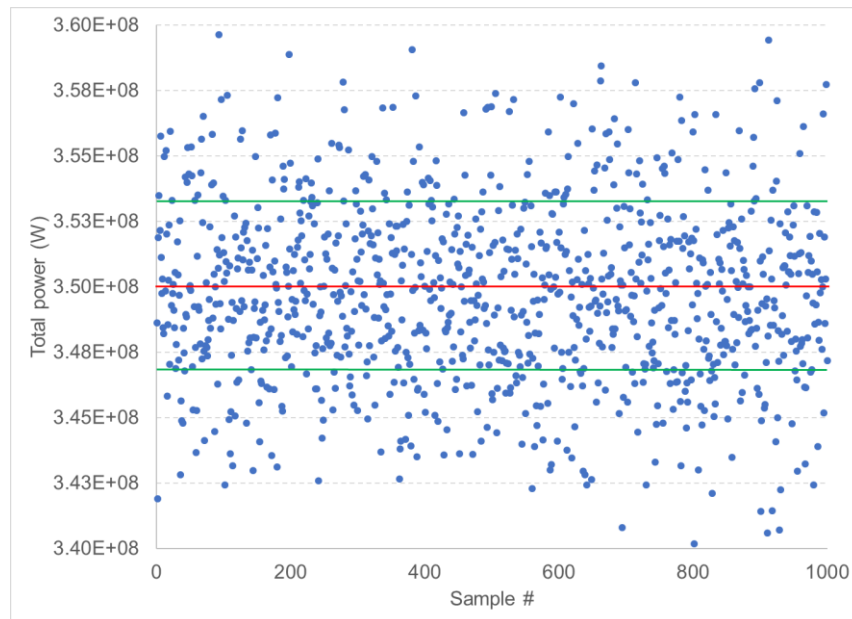


Figure 7-5. Sample scatter plot for total core power (W)

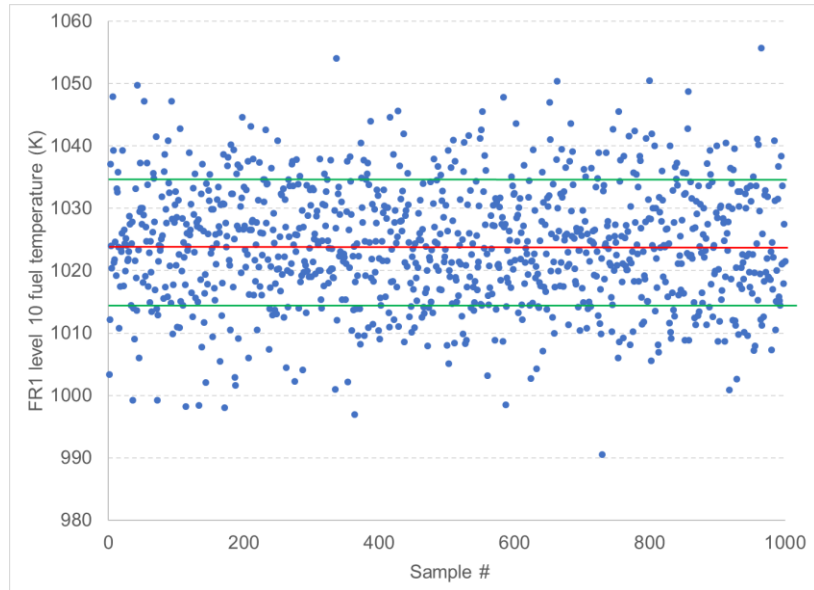


Figure 7-6. Output: Maximum fuel temperature (FR1 level 10) (no bypass)

Table 7-4. Exercise II-4 fuel temperature data for the 0% and 11% bypass flow steady-states

| Axial Level           | Mean fuel temperature (K) |     |     | Standard deviation $\sigma$ (%) |      |      | 95 <sup>th</sup> percentile (K) |     |     |
|-----------------------|---------------------------|-----|-----|---------------------------------|------|------|---------------------------------|-----|-----|
|                       | FR1                       | FR2 | FR3 | FR1                             | FR2  | FR3  | FR1                             | FR2 | FR3 |
| With 11% bypass flows |                           |     |     |                                 |      |      |                                 |     |     |
| 1                     | 519                       | 450 | 460 | 0.74                            | 0.77 | 0.76 | 525                             | 456 | 465 |
| 2                     | 631                       | 525 | 545 | 0.77                            | 0.76 | 0.75 | 639                             | 532 | 552 |
| 3                     | 722                       | 588 | 614 | 0.81                            | 0.77 | 0.77 | 732                             | 595 | 621 |
| 4                     | 791                       | 637 | 667 | 0.84                            | 0.79 | 0.79 | 802                             | 645 | 676 |
| 5                     | 847                       | 678 | 709 | 0.87                            | 0.82 | 0.81 | 859                             | 687 | 719 |
| 6                     | 890                       | 707 | 739 | 0.89                            | 0.83 | 0.82 | 903                             | 717 | 749 |
| 7                     | 931                       | 737 | 769 | 0.90                            | 0.85 | 0.83 | 945                             | 747 | 779 |
| 8                     | 968                       | 763 | 796 | 0.91                            | 0.87 | 0.85 | 983                             | 774 | 807 |
| 9                     | 1000                      | 785 | 817 | 0.92                            | 0.89 | 0.85 | 1015                            | 796 | 828 |
| 10                    | 1024                      | 802 | 831 | 0.93                            | 0.90 | 0.86 | 1039                            | 813 | 843 |
| Zero bypass flows     |                           |     |     |                                 |      |      |                                 |     |     |
| 1                     | 511                       | 446 | 463 | 0.76                            | 0.79 | 0.77 | 518                             | 453 | 469 |
| 2                     | 613                       | 515 | 545 | 0.78                            | 0.77 | 0.75 | 622                             | 522 | 553 |
| 3                     | 695                       | 571 | 611 | 0.82                            | 0.78 | 0.77 | 705                             | 579 | 619 |
| 4                     | 758                       | 615 | 661 | 0.85                            | 0.80 | 0.79 | 769                             | 624 | 671 |
| 5                     | 809                       | 651 | 702 | 0.88                            | 0.82 | 0.81 | 822                             | 661 | 712 |
| 6                     | 848                       | 677 | 731 | 0.90                            | 0.84 | 0.82 | 861                             | 687 | 741 |
| 7                     | 885                       | 704 | 760 | 0.91                            | 0.85 | 0.84 | 900                             | 714 | 771 |
| 8                     | 919                       | 727 | 786 | 0.93                            | 0.87 | 0.85 | 934                             | 738 | 798 |
| 9                     | 948                       | 746 | 807 | 0.94                            | 0.88 | 0.86 | 964                             | 758 | 819 |
| 10                    | 971                       | 761 | 822 | 0.95                            | 0.89 | 0.86 | 987                             | 773 | 834 |

In addition to the mean and standard deviation indicators, Table 7-4 also includes the 95<sup>th</sup> percentile fuel-temperature values, which could be of interest during the assessment of design margin—e.g. the margin available to an operational fuel temperature limit of 1,200 K. If the data in the two tables are compared, two main trends can be observed:

- The addition of bypass flows to the RELAP5-3D model resulted in significantly higher mean fuel temperatures because 11% ( $\pm 1\%$ ) less flow through the fuel region removes less heat through forced convection. The fuel temperature differences between the models with and without bypass flows are lowest in the upper-inlet region of the core (0.8–1.5% in the first axial level), and reach a peak difference value of 5.2% at the core-outlet region (FR1 and Fuel Ring 2 (FR2), Level 10). This increased difference between the two models can be seen in Figure 7-7, where a comparison of the mean and 95<sup>th</sup> percentile FR1 fuel temperatures is shown. The axial profiles of the three fuel rings are shown in Figure 7-8 of the 0% bypass flow model. The inner fuel ring is substantially hotter than the central and outer fuel rings due to MHTGR-350 core loading and lack of central-reflector cooling, but the rise in fuel temperatures down the axial core height is similar.
- In contrast to this trend, the fuel temperature uncertainty ( $\sigma$ ) only increases from 0.7 to 0.9% from the top to the bottom of the core, i.e. *the relative uncertainties in steady-state fuel temperatures are not temperature dependent*. Second, it can also be seen that there is almost no difference in the fuel-temperature uncertainties of the models with and without bypass flows.

The inclusion of bypass flows in the steady-state MHTGR-350 model therefore has a significant impact on the fuel temperatures, but no impact on fuel-temperature uncertainties. This implies that uncertainties in the other input parameters are responsible for the uncertainties in the fuel temperature—an observation that will be confirmed in Section 7.4.2, where the results of the sensitivity study are discussed.

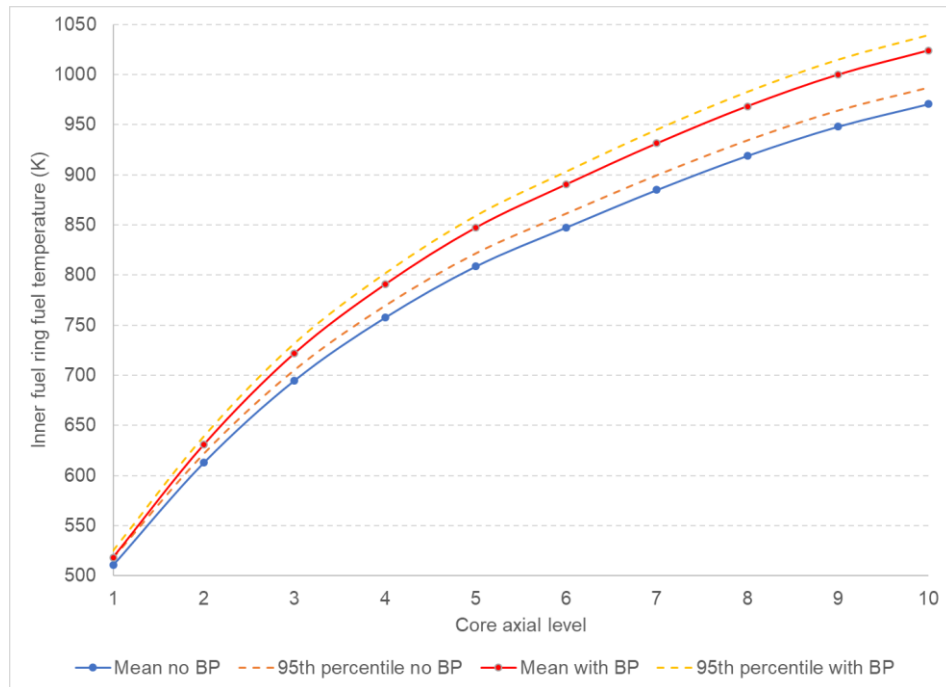


Figure 7-7. Comparison of steady-state mean and 95<sup>th</sup> percentile FR1 axial fuel temperature (K) profiles for the models with 11 and 0% bypass flows.

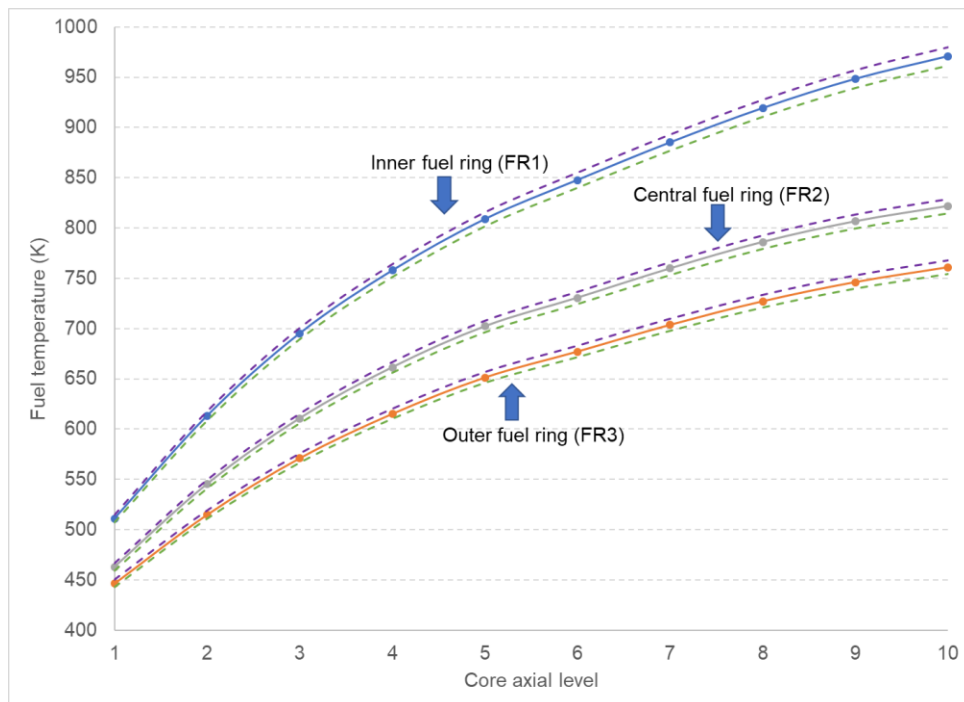


Figure 7-8. Comparison of FR1, FR2, and Fuel Ring 3 (FR3) mean and standard-deviation fuel temperatures for the 0% bypass model.

### 7.4.2 Exercise II-4 Sensitivity Results

For the sensitivity assessment, RAVEN is once again used to calculate typical sensitivity indicators based on the sample population. Following the general approach introduced in Chapter 3, the RAVEN PCCs are used as a first screening to assess whether a significant degree of linear correlation exists between the input parameters and the MFT as main FOM. PCC values larger than  $R^2 = 0.01$  are typically indicative of a meaningful degree of linear correlation, and the sensitivity coefficients determined by RAVEN can be used for a ranking assessment. On the other hand, PCC values less than 0.01 indicate weak or no linear-correlation dependencies, and the sensitivity coefficients can potentially contain large uncertainties.

A comparison of the ranked PCCs obtained for the two bypass-flow models is presented in Table 7-5, and visually in Figure 7-9 and Figure 7-10. Regardless of the inclusion of bypass flows in the two models, the highest-ranked parameters by a large margin are total power, inlet mass-flow rate, and inlet-gas temperature. The signs of the PCCs indicate the relationship between the parameter and the MFT; e.g. the PCC value of -0.668 indicates that there is a strong linear dependency between the mass-flow rate and the MFT, and specifically that a decrease in mass-flow rate would increase the MFT.

Following the top three ranked boundary-condition parameters, the graphite H-451 core thermal conductivity is ranked fourth, with the first of the bypass flows in the fifth-ranked position. (The labels of the bypass-flow channels were provided in Table 7-1.) With the exception of the core-barrel and reflector thermal conductivities, all input parameters listed in Table 7-5 are above the  $R^2 = 0.01$  criterion, but only the top three input parameters are strongly linearly correlated. This ranking is similar to the findings of the PBMR-400 study performed by the author with the TINTE code (Strydom 2004), in which a simple brute-force sensitivity study identified the top four input-parameter sensitivities as total power, fuel thermal conductivity, reactor inlet mass-flow rate, and helium-inlet temperature.

The relative magnitude of the bypass-flow PCCs and the lack of impact on the PCC ranking order both confirm the preliminary conclusion made in Section 7.4.1 that the inclusion of bypass-flow uncertainties, and even the inclusion of *any* bypass-flow channels, is not important for the determination of MFT *uncertainties*. (As stated before, the inclusion of bypass flow remains very important for *nominal* MFT estimates, and a larger uncertainty range should also be assessed in future work).

Table 7-5. Comparison of Exercise II-4 PCCs for the 0 and 11% bypass-flow models.

| Parameter             | 11% bypass flow |      | 0% bypass flow |      |
|-----------------------|-----------------|------|----------------|------|
|                       | PCC             | Rank | PCC            | Rank |
| Total power           | 0.679           | 1    | 0.663          | 2    |
| Inlet flow rate       | -0.668          | 2    | -0.671         | 1    |
| Inlet gas temperature | 0.289           | 3    | 0.35           | 3    |
| H451_core_k           | -0.077          | 4    | -0.08          | 4    |
| Bypass_500            | -0.052          | 5    | -              | -    |
| Bypass_600            | -0.051          | 6    | -              | -    |
| Refl_rho_cp           | -0.041          | 7    | -0.028         | 10   |
| RPV_k                 | 0.041           | 8    | 0.0547         | 5    |
| Fuel_k                | -0.040          | 9    | 0.0552         | 6    |
| Bypass_650            | -0.039          | 10   | -              | -    |
| Bypass_210            | -0.037          | 11   | -              | -    |
| Bypass_400            | -0.035          | 12   | -              | -    |
| Bypass_700            | -0.033          | 13   | -              | -    |
| Bypass_300            | 0.029           | 14   | -              | -    |
| H2020_refl_k          | -0.015          | 15   | 0.037          | 8    |
| Bypass_230            | 0.013           | 16   | -              | -    |
| Bypass_200            | 0.011           | 17   | -              | -    |
| Fuel_rho_cp           | -0.010          | 18   | -0.021         | 11   |
| CB_k                  | 0.009           | 19   | -0.030         | 9    |
| H451_refl_k           | -0.008          | 20   | -0.039         | 7    |

While the PCC data can be used to assess the degree of linear correlation between the input and output parameters, the NSCs can be used to quantify the sensitivity of the MFT to changes in a specific input parameter. In RAVEN, the least-square correlation sensitivity indices are simply defined as the relationship of an input parameter to the standard deviation  $\sigma$  of the FOM—i.e. in this case, to what degree a specific input parameter impacts the MFT  $\sigma$ <sup>44</sup>. The normalized version of these sensitivity-coefficients values allows direct comparisons between parameters that vary significantly in absolute terms, e.g. the total power is perturbed by 3.5E+06 W, while the thermal conductivity is perturbed by 4 W/m.K.

<sup>44</sup> The mathematical definitions of these sensitivity metrics are included in Appendix E2.

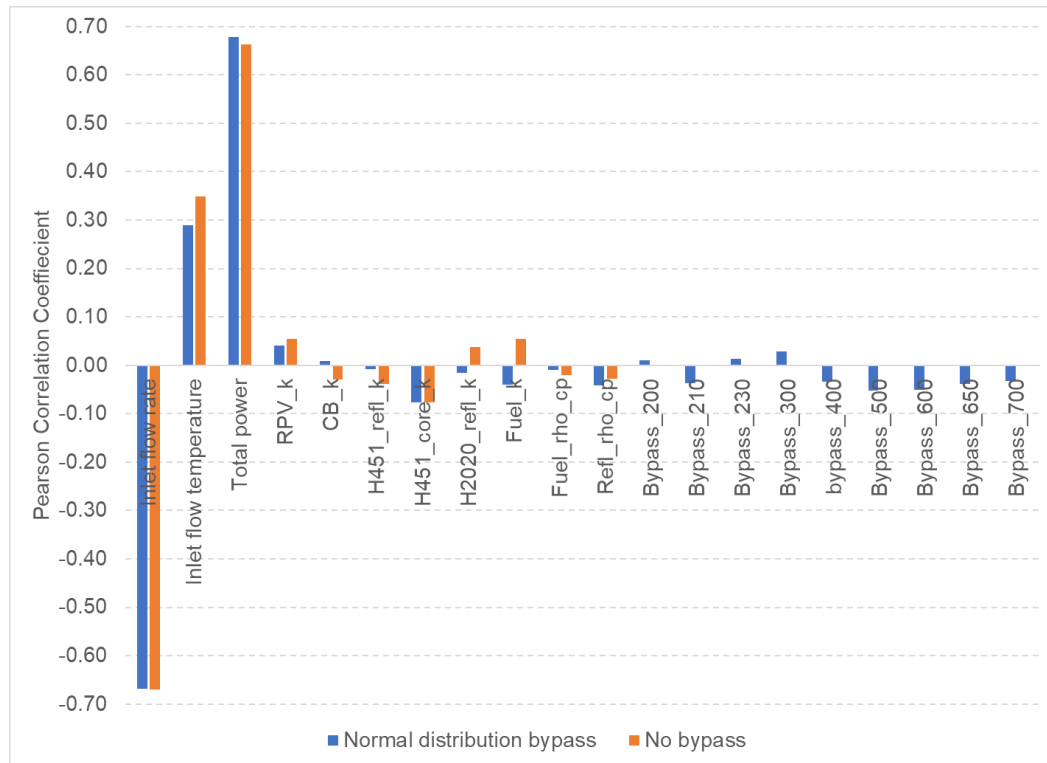


Figure 7-9. Comparison of steady-state MFT PCCs for models with and without bypass flows.

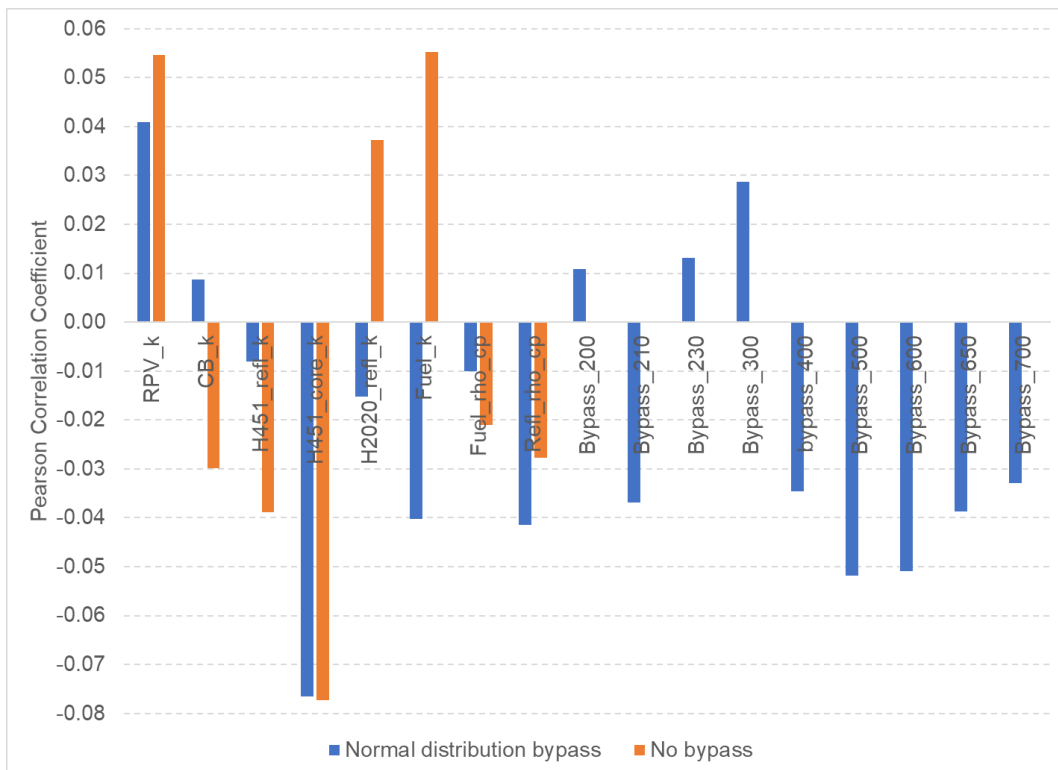


Figure 7-10. Detail of the lower-ranked steady-state MFT PCCs for models with and without bypass flows.

The NSC data shown in Table 7-6 indicate that the three boundary-condition input parameters again occupy the top three rankings for both the 0 and 11% model versions with NSC values above 0.25, or almost a factor of 200 above the fourth-ranked input parameter. In fact, because most of the PCC values for the lower-ranked input parameters are less than 0.05, the uncertainties in the NSC values smaller than 0.01 are relatively high, implying that most of the relative rankings in Table 7-6 below the fifth place should be classified in the “not-so-important” category. The only bypass flow included in the top 10 ranking is the flow in bypass channel 300 that is coupled to the inner FR1 core flow<sup>45</sup>, confirming the insignificant contributions of bypass flows in general to the steady-state MFT uncertainties.

Table 7-6. Comparison of Exercise II-4 normalized sensitivity coefficients for the 0 and 11% bypass-flow models.

| Parameter             | With bypass flow |      | No bypass flow |      |
|-----------------------|------------------|------|----------------|------|
|                       | NSC              | Rank | NSC            | Rank |
| Total power           | 0.6461           | 1    | 0.6337         | 1    |
| Inlet flow rate       | -0.6368          | 2    | -0.6273        | 2    |
| Inlet gas temperature | 0.2770           | 3    | 0.3396         | 3    |
| RPV_k                 | 0.0151           | 4    | 0.0207         | 4    |
| Bypass_300            | 0.0105           | 5    | -              |      |
| H451_core_k           | -0.0102          | 6    | -0.0101        | 6    |
| Refl_rho_cp           | -0.0077          | 7    | -0.0052        | 11   |
| Fuel_k                | -0.0053          | 8    | 0.0074         | 8    |
| CB_k                  | 0.0033           | 9    | -0.0111        | 5    |
| Fuel_rho_cp           | -0.0032          | 10   | -0.0067        | 10   |
| H2020_refl_k          | -0.0028          | 11   | 0.0069         | 9    |
| Bypass_500            | -0.0016          | 12   | -              |      |
| H451_refl_k           | -0.0015          | 13   | -0.0079        | 7    |
| Bypass_600            | -0.0014          | 14   | -              |      |
| bypass_400            | -0.0011          | 15   | -              |      |
| Bypass_650            | -0.0011          | 16   | -              |      |
| Bypass_700            | -0.0010          | 17   | -              |      |
| Bypass_210            | -0.0009          | 18   | -              |      |
| Bypass_230            | 0.0004           | 19   | -              |      |
| Bypass_200            | 0.0003           | 20   | -              |      |

<sup>45</sup> This example illustrates the difference between PCC and NSC metrics. Bypass\_300 is ranked 14<sup>th</sup> on the PCC metric, indicating a weak linear relationship (the non-linear nature of bypass-flow impact on fuel temperature is already known). But it is ranked above all other bypass flows in terms of NSC actual impact on MFT variance, and its higher rank matches well with the physical location of this bypass-flow channel. Based on first principles, this bypass flow *should* be more important than any other bypass flow because it is directly coupled to the MFT node.

## 7.5 Exercise IV-1: Pressurized Loss of Forced Cooling

The coupling between the steady-states created for Exercise II-4 and the PLOFC transient defined for Exercise IV-1 is indicated in Figure 7-4. The PLOFC event is typically initiated by a turbine trip (Strydom 2015) that results in the forced mass flow decreasing linearly down to 0.0 kg/s over 30 seconds. Because only the changes in the thermal response of the core are of interest, and the transient is performed with coupling to the neutron kinetics, no control-rod movements are defined for this transient.

The 1,000 perturbed converged steady-states of Exercise II-4 are used as the starting points for 1,000 PLOFC transient simulations by utilizing the standard restart capability of RELAP5-3D. The only additional parameter introduced in the PLOFC simulation is the perturbation of the decay-heat multiplication factors, as described in Section 7.3. Decay heat only plays a role after the control rods have been inserted using a trip function in RELAP5-3D. Because the PLOFC with inserted control rods is a subcritical transient, this simulation does not require feedback to and from the PHISICS neutron-kinetics module, and the stand-alone thermal fluid approach taken for Exercise II-4 can also be applied to the PLOFC transient. As indicated before, the current calculation sequence is designed to isolate the contributions from thermal fluid parameters, and the impact of cross-section uncertainties on the steady-state and PLOFC MFTs is not quantified.

The two models developed in the previous section to assess the impact of bypass flows are used again to perform an uncertainty and sensitivity assessment of the PLOFC event because the physical phenomenon that dominated the steady-state (convective heat transfer via forced helium flow) is not present during the loss-of-cooling transient. As an application of the statistical U/SA methodology to one of the most-important safety-case transients for HTGRs, the objective of this section is to calculate time-dependent uncertainty indicators and to identify the main contributors to the MFT uncertainty.

### 7.5.1 Exercise IV-1 Uncertainty Results

During a loss-of-cooling event, a transition occurs within the first few minutes between the high-velocity downward-forced convective heat transfer and the low-velocity, upwards, buoyancy-driven natural convection-flow regimes. This change in flow pattern distributes decay heat from the fuel to the colder regions in the upper part of the core, and eventually the fuel-temperature axial profile mirrors the core power profile, with the location of the MFT moving upwards by several meters. The change in the axial mean FR1 fuel-temperature profile is shown in Figure 7-11 at 0.45 hours and 24 hours after the start of the PLOFC, in addition to the change in the FR1 fuel-temperature standard deviation.

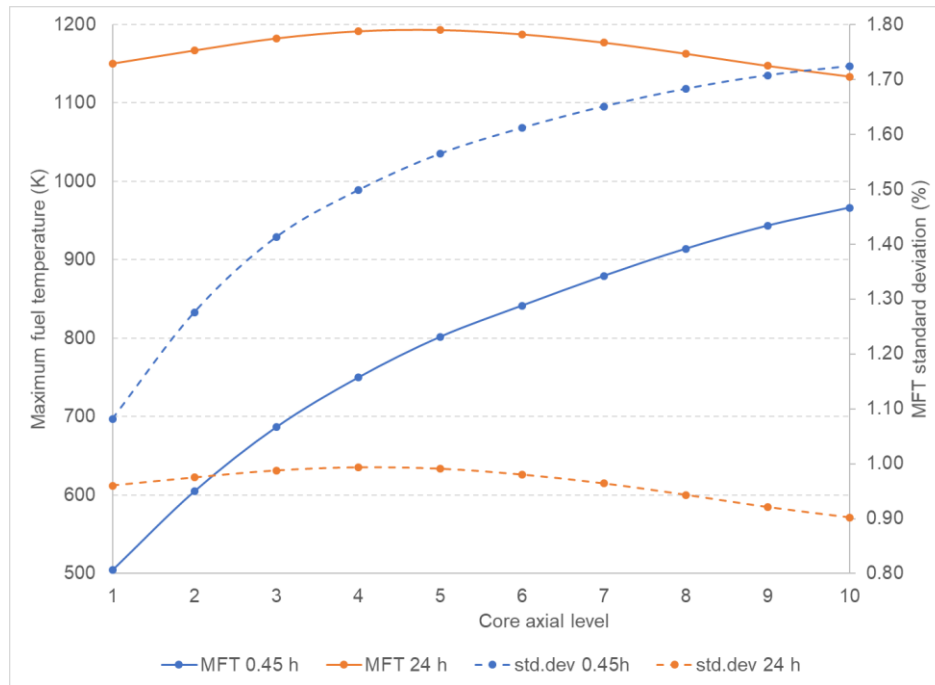


Figure 7-11. Change in axial mean and standard deviation FR1 profiles between 0.45 h and 24 h.

The significant redistribution of heat upwards in the core can be seen by comparing the much-flatter temperature profile at 24 hours with the peaked axial profile at 0.45 hours. The standard deviation of these mean-temperature profiles shows the same flattening over time, but it is interesting to note that, in relative percentage terms, the standard deviation is less at 24 hours than at 0.45 hours.

From the two examples shown in Figure 7-11, it should be clear that the location of the MFT moved from the bottom of the core (Level 10) at 0.45 hours to the midpoint of the core (Axial Level 5). This implies that, for the MFT PLOFC data shown in Figure 7-12, the locations of these “peak” fuel temperature points change as a function of time, especially during the first 10–15 hours of the PLOFC. The MFT trends in Figure 7-12 follow the typical HTGR behaviour of first sharply cooling down due the rapid decrease in fission-power generation, but then turning around within ~30 minutes to start the ~30-hour heating phase as decay heat generates more energy than can be transported out of the core with natural convection.

Due to the large heat capacity of graphite, the cooling phase (when decay-heat generation is less than heat removal through natural convection) is a very slow process; in the case of this MHTGR-350 design, the MFT decreases by less than 100 K over the final 60 hours.

MFT data in Figure 7-12 are shown for the first 200 perturbations of the 0% bypass-flow model, in addition to a focus on the period between 5–65 hours (Figure 7-13). In the latter figure, it can be seen that the timing of the peak MFT (i.e. the turnaround point) is only influenced weakly by the uncertainties in the sampled input parameters; most PLOFC transients reach turnaround in  $25 \pm 5$  hours.

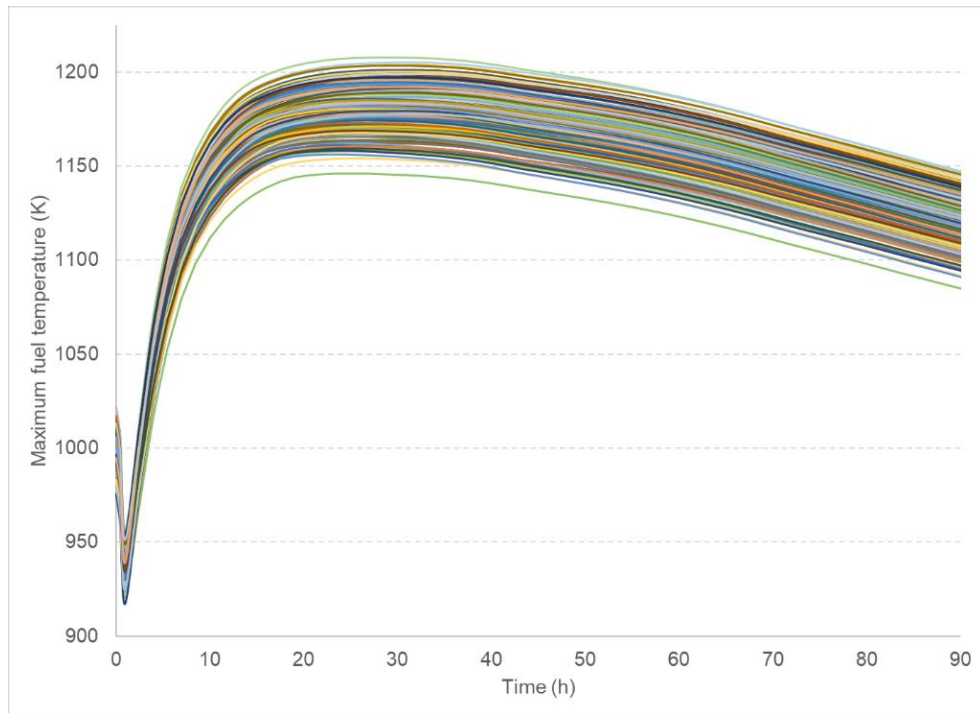


Figure 7-12. MFT (K) values for perturbed samples 1–200 of the 0% bypass flow model.

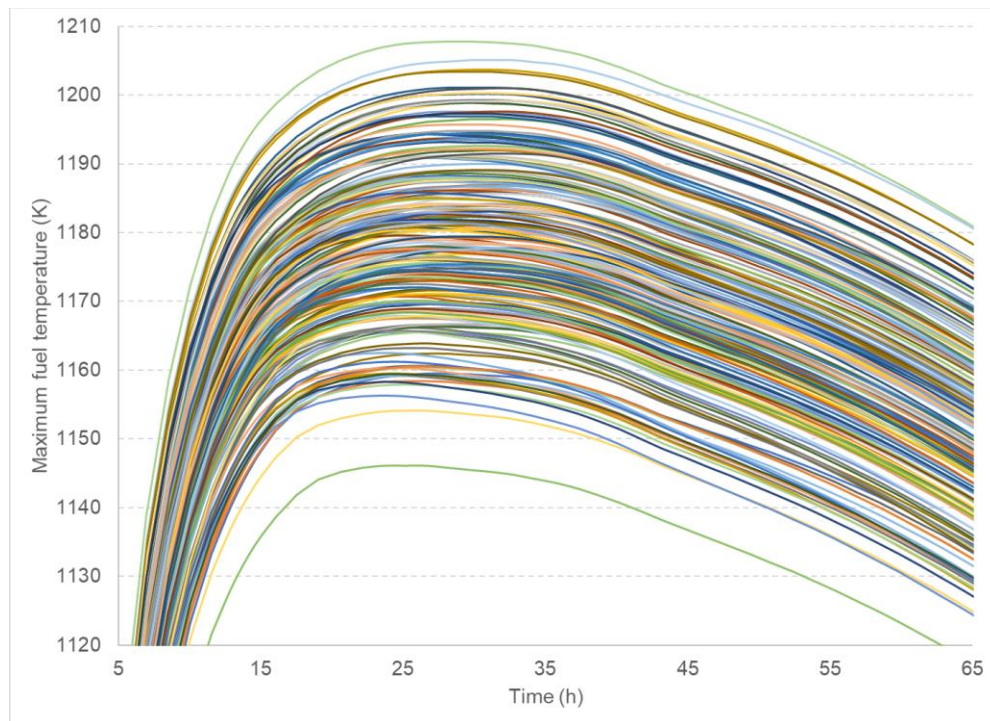


Figure 7-13. MFT (K) values for perturbed samples 1–200 of the 0% bypass flow model—detail between 5–65 h.

The MFT mean and standard-deviation values for the full set of 1,000 perturbations is presented in Figure 7-14 and Figure 7-15, respectively. The MFT data sets are shown for both the 0 and 11% bypass flow models. As shown in Figure 7-3 for the mean MFT values, the addition of bypass flows leads to significantly lower and delayed peak MFT values.

The change in the MFT standard deviation in absolute (K) and relative (%) units is shown in more detail in Figure 7-16 and Figure 7-17, where the impact of the bypass flows are again shown to be minimal. For both data sets the MFT standard deviation starts off at the highest value (e.g. 18.5 K or 1.76% for the 11% bypass model) and decrease to between 10 and 13 K (0.9–1.2%) for the duration of the PLOFC transient. In relative terms (i.e.  $100 \times \sigma/\mu$ ), the MFT uncertainties for the PLOFC are larger than the steady-state values discussed in Section 7.4.1 due to the addition of decay-heat uncertainties. The largest differences between the two models with and without bypass flow occur at the start and end of the PLOFC, but the MFT  $\sigma$  uncertainties remain within 0.15% for both data sets.

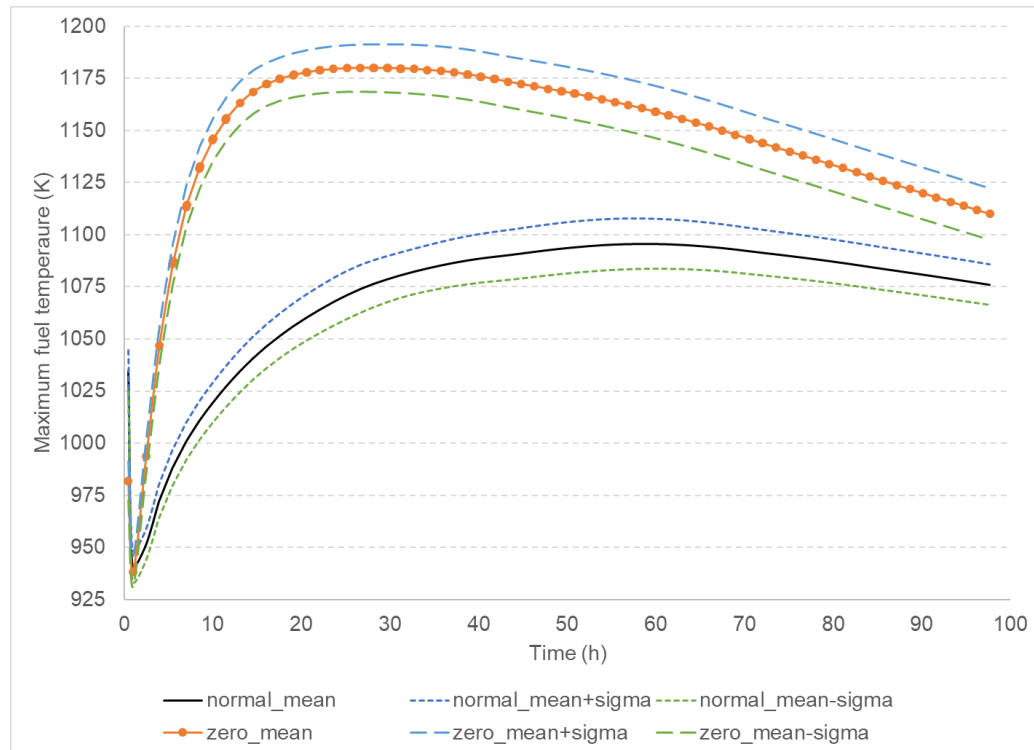


Figure 7-14. Comparison of MFT mean and  $\pm\sigma$  values for the 0 and 11% bypass-flow models.

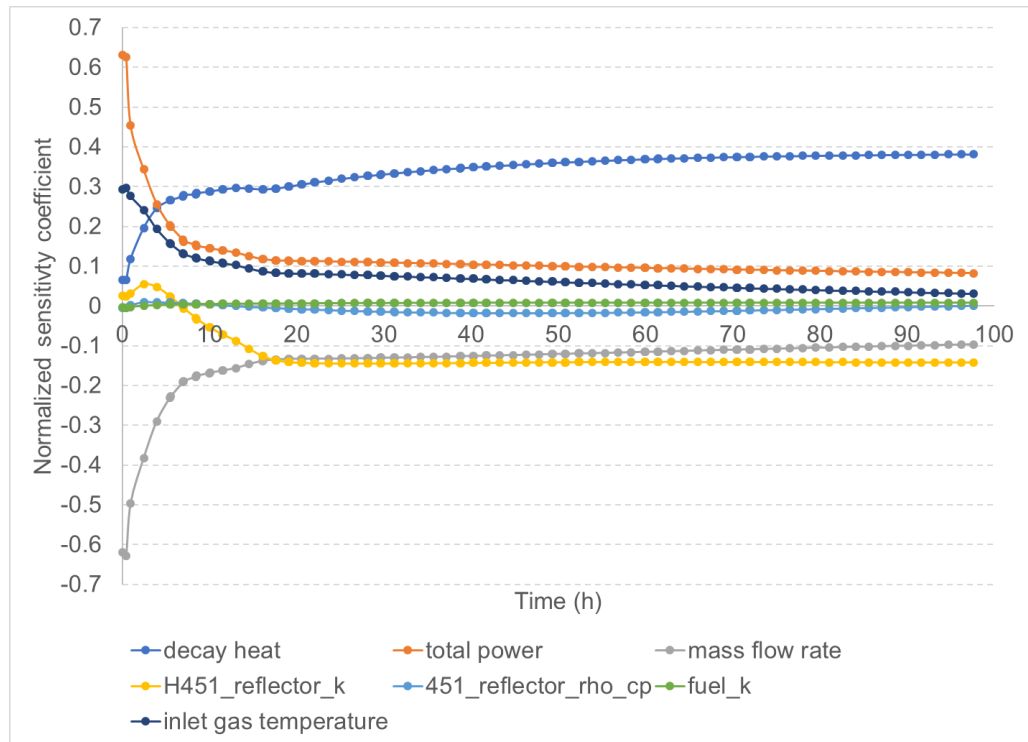


Figure 7-15. Comparison of MFT NSC values for the 0% bypass-flow model.

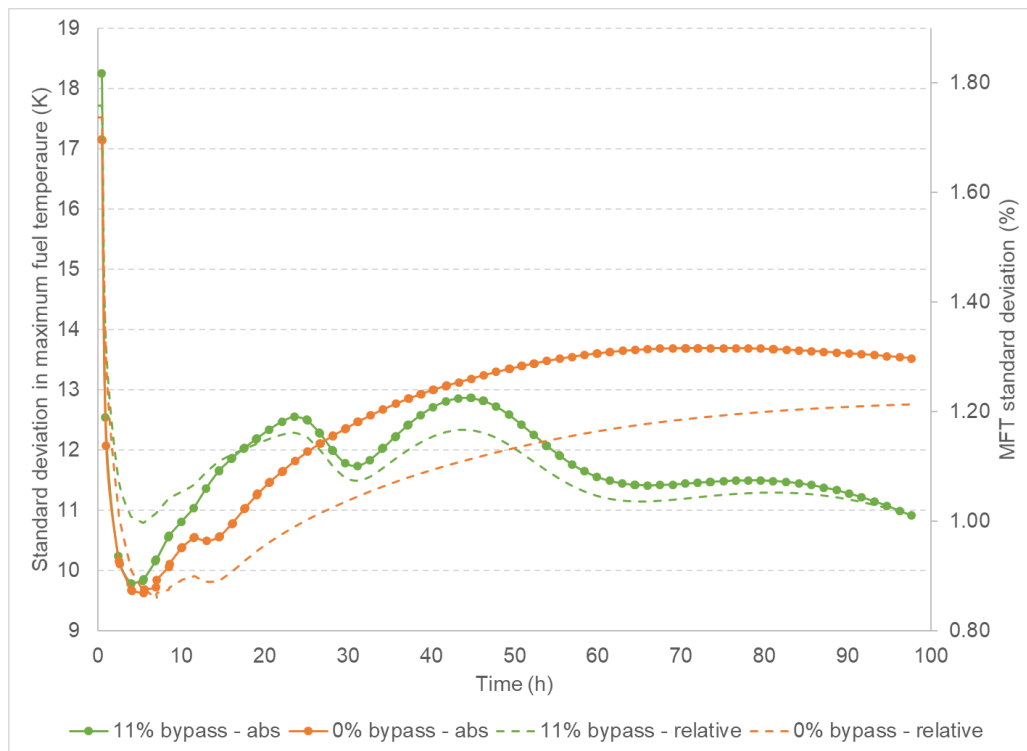


Figure 7-16. Comparison of absolute and relative MFT  $\sigma$  for the 0 and 11% bypass-flow models.

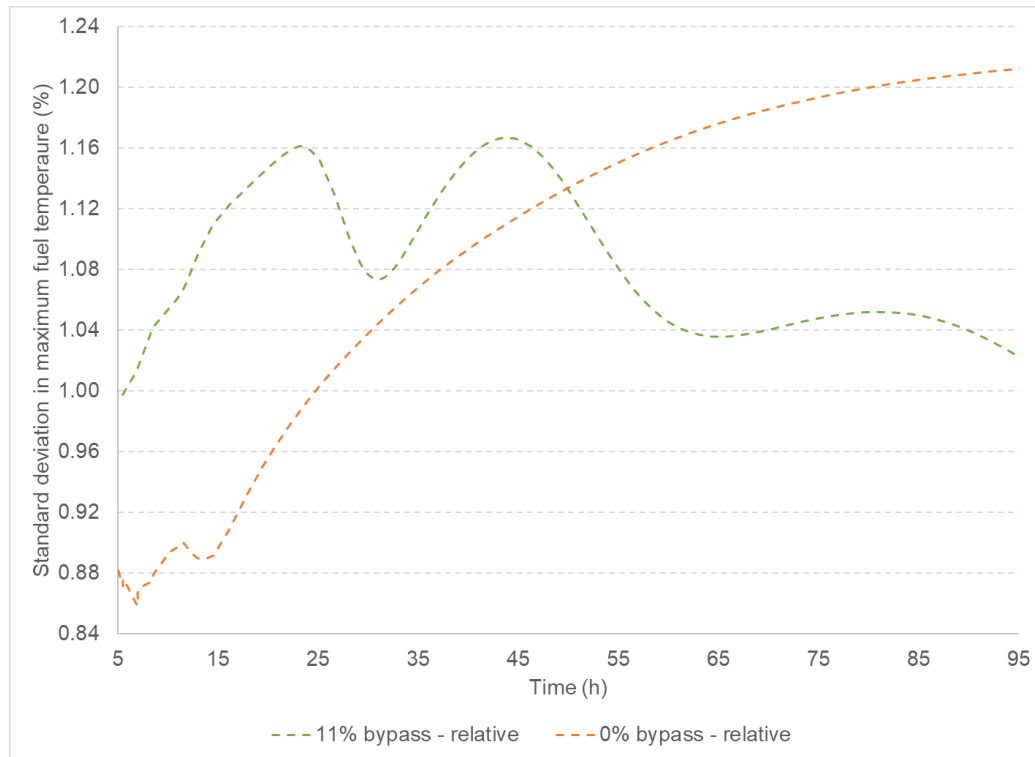


Figure 7-17. Detail of the relative MFT  $\sigma$  for the 0 and 11% bypass-flow models between 5–95 hours.

### 7.5.2 Exercise IV-1 Sensitivity Results

Time-dependent PCCs for the PLOFC MFT with 0 and 11% bypass flows are shown in Figure 7-18 and Figure 7-19, respectively. The data are representative of the change in dominant physical phenomena over the duration of the PLOFC. During the first three hours, the three steady-state boundary-condition parameters (total power, inlet-gas flow rate and inlet-gas temperature) retain their dominant rankings (first, second and third, respectively), but as shown in Figure 7-20, the degree of linear correlation of decay-heat uncertainties with the MFT surpasses all other factors after approximately three hours. It continues to rise to an almost completely fully correlated variable at the end of the PLOFC.

The influence of three steady-state boundary-condition parameters continuously decline as the PLOFC progresses, and all three are surpassed by the reflector-graphite thermal conductivity as the second ranked input parameter after 35 hours of the model with no bypass flows. For the model with 11% bypass flows, the reflector's specific-heat capacity ranks even higher than thermal conductivity during certain time points of the PLOFC (see Figure 7-19 for detail). With more than 600 tons of graphite material in the reflector structures, uncertainties in both the reflector's thermal conductivity and specific-heat capacity could be expected to play significant roles in the later stages of the PLOFC.

The PCC for the most-significant bypass flow (bypass\_300 in FR1) is also included in Figure 7-21, where the weak correlation can again be observed.

The conclusion reached for the steady-state Exercise II-4 is again confirmed for the PLOFC transient: the addition of bypass flows did not change the main sensitivity drivers of uncertainty, and the treatment of bypass-flow uncertainties is not important if the FOM is the MFT. For safety-critical components like the control-rod drives located in the side reflector, however, the assessment of local temperatures could be significantly affected by the variances in local-bypass flows. Likewise, peak reactor-vessel or core-barrel temperatures during the PLOFC were not investigated in the scope of this work. It can be postulated that variances in the large leak flow between the side reflector and the barrel, for example, can lead to local impacts on the barrel axial-temperature profile that would be the subject of typical safety-case assessments. Because the same statistical methodology illustrated in this chapter can be applied to target multiple component FOMs, this approach could be an asset for HTGR core designers and regulators.

The trends observed for the MFT normalized sensitivity coefficients presented in Figure 7-22 confirm the earlier ranking of the input parameters based on the PCCs. Approximately ten hours into the PLOFC event, decay-heat uncertainty dominates all other input-parameter uncertainties, followed by the H-451 reflector graphite's thermal conductivity and the inlet mass-flow rate in the second and third positions after ~50 hours. The more prominent role of H-451 reflector-graphite thermal conductivity in the 0% bypass flow model is likewise apparent; i.e. the hotter reflector has a larger impact (-0.15) on the MFT uncertainties than the colder reflectors' role in the model with 11% bypass flows (-0.05).

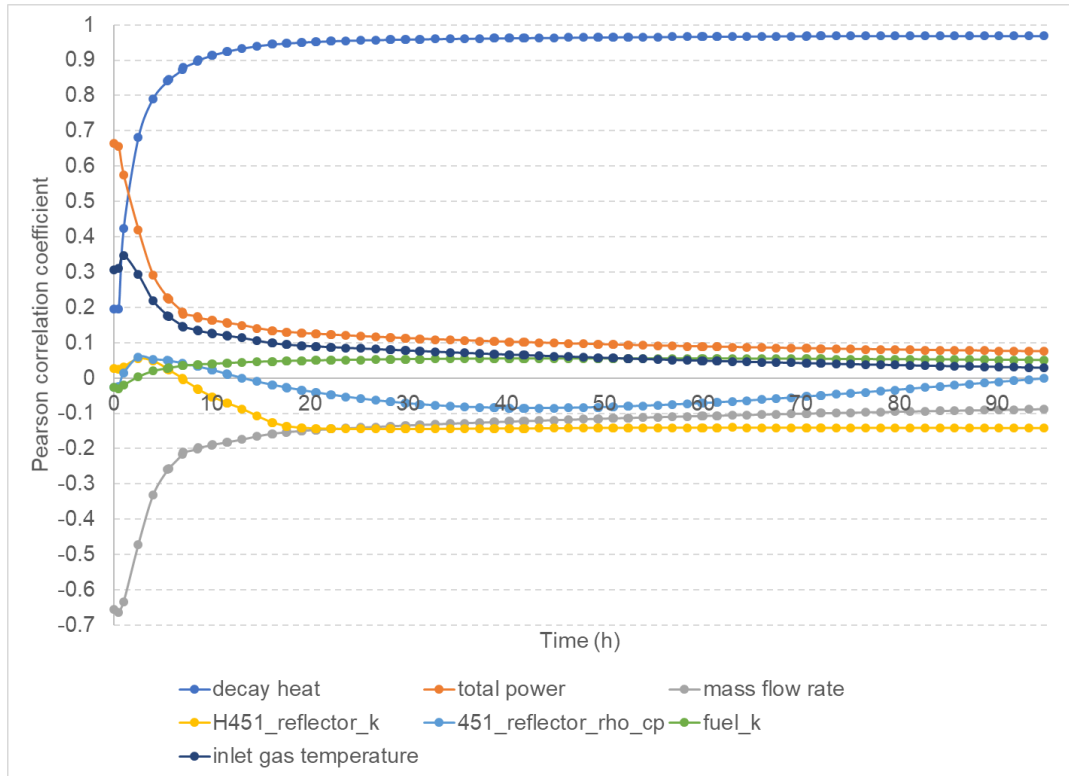


Figure 7-18. Comparison of MFT PCC values for the 0% bypass flow model.

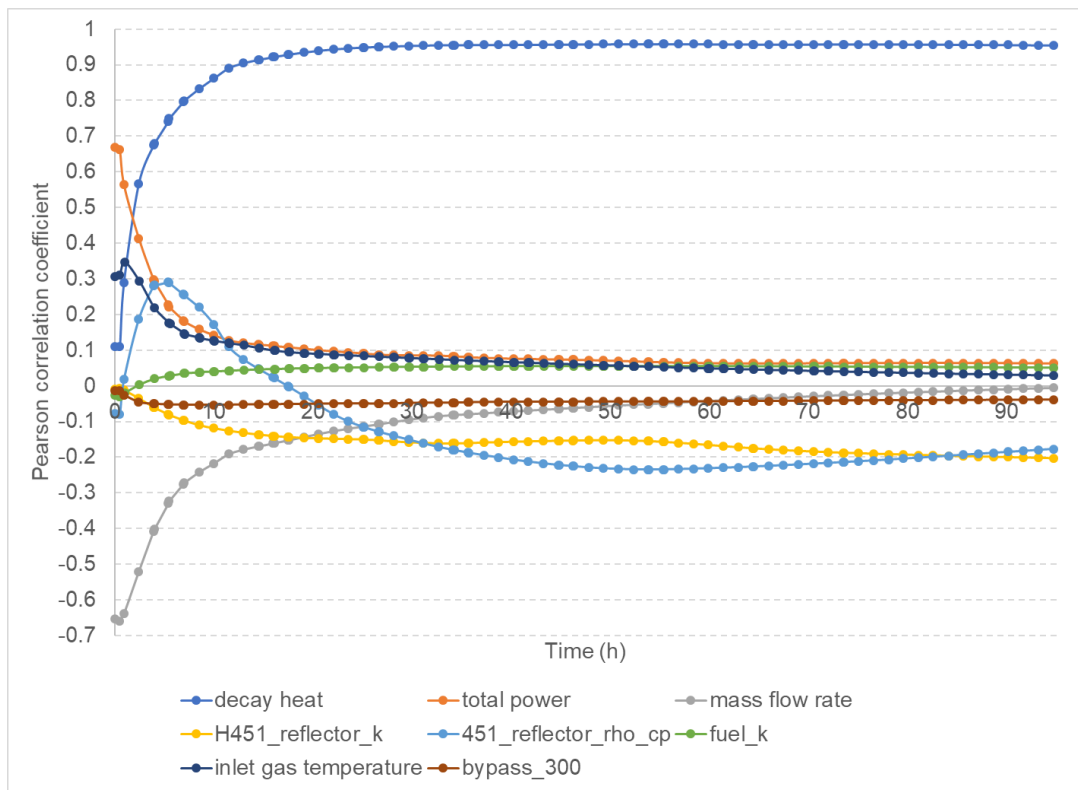


Figure 7-19. Comparison of MFT PCC values for the 11% bypass flow model.

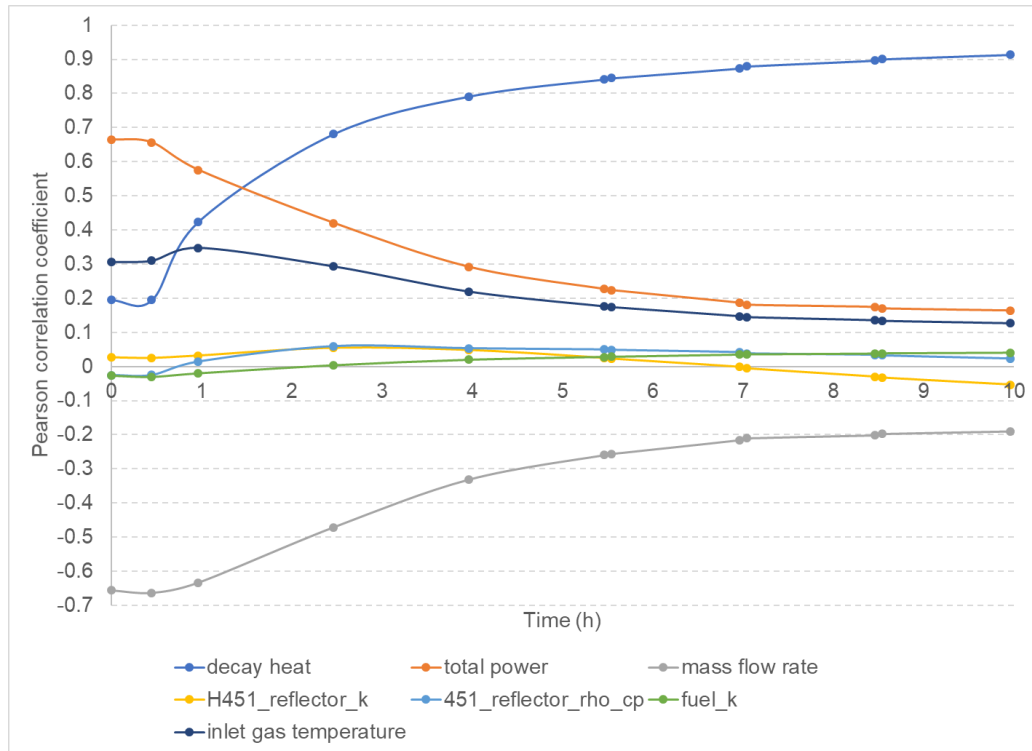


Figure 7-20. Comparison of MFT PCC values for the 0% bypass flow model: detail of the first ten hours.

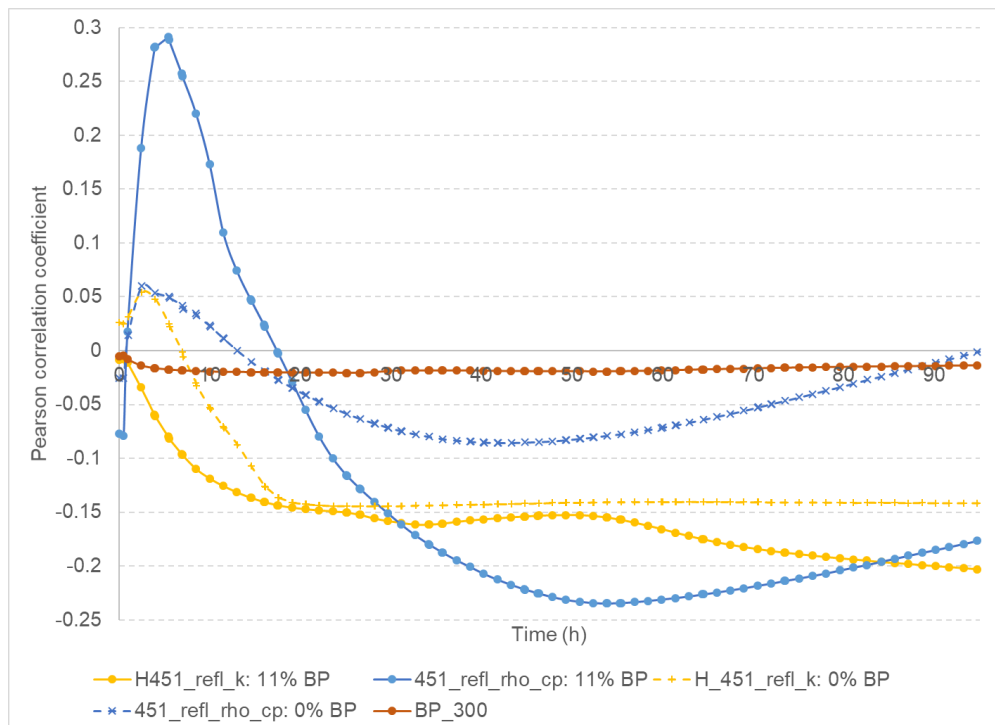


Figure 7-21. Comparison of MFT PCC values for H-451 reflector graphite in the 0 and 11% bypass flow models.

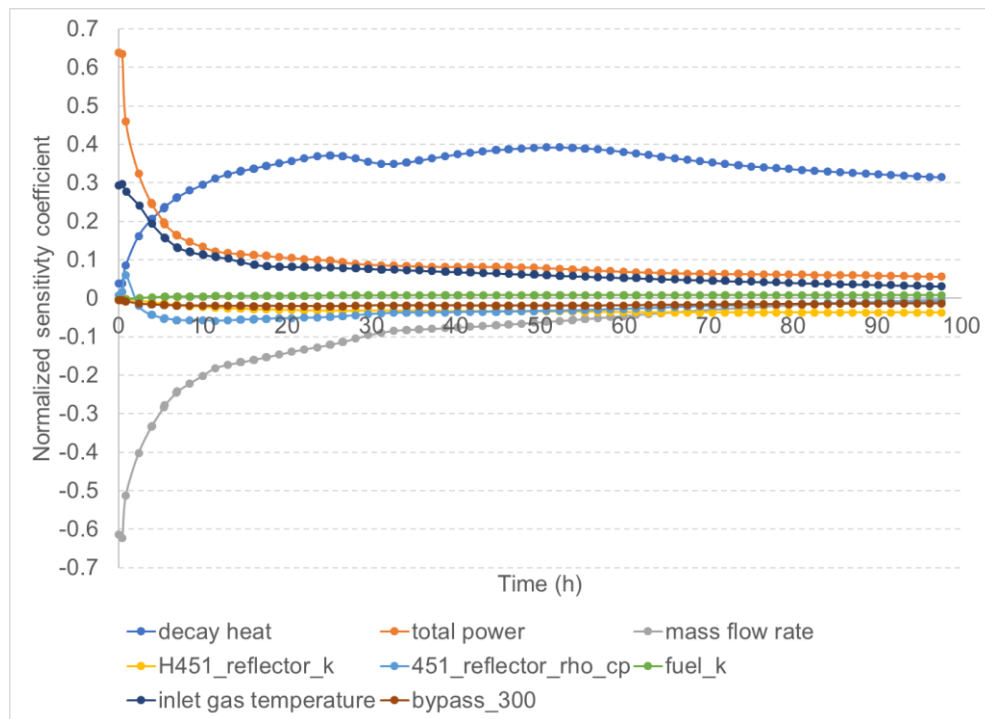


Figure 7-22. Comparison of MFT NSC values for the 11% bypass flow model.

## 7.6 Conclusion

The objective of Chapter 7 is an uncertainty and sensitivity assessment of the two exercises defined for the stand-alone thermal fluids core steady-state, Exercise II-4, and the PLOFC transient, Exercise IV-1. The stand-alone core thermal fluid exercises are designed to isolate the impact of input uncertainties in thermal fluid boundary conditions and material properties, and do not include any feedback to reactor neutronics. This chapter constitutes one of the major contributions of the author to the IAEA CRP on HTGR UAM—all other contributions so far focused on cross-section and material uncertainty assessments—and represents the first application of the statistical-sampling methodology on HTGR core thermal fluids simulations.

As input to the RAVEN/RELAP5-3D sampling methodology, five boundary condition and six material-property input parameters were selected to be perturbed, based on distribution data in the literature. A specific focus of this chapter was the uncertainty assessment of bypass flows (i.e. helium flow that bypasses the fuel-block coolant channels), which is another unique contribution to the IAEA CRP. Two approaches were introduced: two discrete models utilizing either a 0 or 11% bypass-flow fraction, and a second method that utilized RAVEN to sample 1,000 perturbed values from normal distributions defined for each of the seven bypass-flow channels.

For the steady-state, Exercise II-4, it was found that the addition of bypass flows to the RELAP5-3D model resulted in significantly higher mean fuel temperatures (up to 5.2%) because 11% less flow through the fuel region removes less heat through forced convection. The fuel temperature uncertainty ( $\sigma$ ), however, only varied between 0.7 and 0.9% from the top to the bottom of the core, i.e. the relative uncertainties in steady-state fuel temperatures are not temperature dependent. It was also found that there is almost no difference in fuel-temperature uncertainties of models with and without bypass flows. The inclusion of bypass flows in the steady-state MHTGR-350 model, therefore, has a significant impact on fuel temperatures, but no impact on fuel-temperature uncertainties.

For the steady-state sensitivity assessment, RAVEN was used to calculate NSCs and PCCs. It was found that, regardless of the inclusion of bypass flows in the two models, the highest-ranked parameters by a large margin are total power, inlet mass-flow rate, and inlet-gas temperature. The impact of the Graphite H-451 core thermal conductivity on the MFT was ranked fourth, with the first of the bypass flows in the fifth-ranked position.

The steady-state defined for Exercise II-4 is artificial in the sense that no coupled feedback exists between the thermal fluid and neutronics modules, but the PLOFC transient defined for Exercise IV-1 is more realistic because the PLOFC event with a control-rod insertion is dominated primarily by thermal fluid phenomena. Due to a transition between the high-velocity downward-forced convective heat transfer and the low velocity, upwards, buoyancy-driven natural convection flow regimes, the axial location of the peak fuel temperature moved upwards by several meters. Both the MFT mean and standard-deviation values varied as a function of time, and the addition of bypass flows leads to significantly lower and delayed peak MFT values. For both models—with and without bypass flows—the MFT standard deviation starts off at the highest value (e.g. 18.5 K or 1.76% for the 11% bypass model) and decreases to between 10 and 13 K (0.9–1.2%) for the duration of the PLOFC transient. In relative terms the MFT uncertainties for the PLOFC are larger than the steady-state uncertainties due to the addition of the decay-heat uncertainties.

For the PLOFC sensitivity assessment, it was found that time-dependent PCC and NSC data reflect changes in the dominant physical phenomena over the duration of the PLOFC. During the first three hours, the three dominant steady-state boundary-condition parameters (total power, inlet gas-flow rate, and inlet-gas temperature) retain their dominant rankings (first, second, and third, respectively), but decay-heat uncertainties surpass all other input uncertainties after approximately three hours. They continue to rise to an almost completely fully correlated variable at the end of the PLOFC. The influence of the three steady-state boundary-condition parameters continuously decline as the PLOFC progresses and are surpassed by the reflector-graphite thermal conductivity as the second ranked input parameter after 35 hours of the model with no bypass flows.

In summary, it was found that the addition of bypass flows did not change the main sensitivity drivers of uncertainty for both the steady-state and the PLOFC transient, and the treatment of bypass-flow *uncertainties* is not important if the FOM is the MFT. The inclusion of bypass flows remains very important for best-estimate analysis and would possibly impact other safety-critical equipment, like the control-rod drives, much more significantly. The fuel-temperature uncertainty varied between 0.7 and 0.9% for the stand-alone steady-state, and up to 1.24% at the end of the PLOFC transient. The main drivers of these uncertainties were uncertainties in the total power, inlet mass-flow rate, inlet-gas temperature, and reflector-graphite conductivity. For the PLOFC, decay-heat uncertainty dominated all other input uncertainties by a large margin.

To assess the effect of coupled feedback between the power and temperature fields, and add the uncertainties in cross-sections from the models generated in Chapter 7.2, these stand-alone thermal fluid results will be compared with the uncertainties and sensitivity data obtained for the coupled neutronics and thermal fluid steady-state and CRW transient in Chapter 8.

## 8. MHTGR-350 EXERCISES III-1 AND IV-2: COUPLED CORE NEUTRONICS AND THERMAL FLUIDS STEADY-STATE AND CRW TRANSIENT

*"Uncertainty" is not "I don't know." It is "I can't know." Werner Heisenberg.*

The results obtained for the propagation of cross-section uncertainties from the MHTGR-350 NEWT lattice models into the core stand-alone P/R models were discussed in Chapter 6 for the eigenvalue, power peaking and other parameters of interest in general core-physics analysis. The impacts of input uncertainties in thermal fluid parameters on the MFT were likewise summarized in Chapter 7 for the stand-alone RELAP5-3D core models. Both of these data sets are artificial in the sense that neutronics and thermal fluids are coupled in any realistic reactor analysis, but the isolation of the separate effects was useful to identify the major contributors to uncertainties in the chosen FOMs without complex feedback effects.

The primary objective of Chapter 8 is the combined uncertainty assessment of both neutronics and thermal fluid input uncertainties for the FOMs targeted in earlier chapters, and the main sensitivity drivers are identified and compared in terms of relative sensitivity and PCC rankings. As secondary objectives, the impact of core-model energy-group boundaries on FOM uncertainties are again investigated by comparing the results obtained for the 2- and 8-group structures introduced in Chapter 6, and by including the Chapter 7 bypass-flow perturbations into the coupled analysis, the relative low importance of this parameter is also confirmed for the coupled core models. The results discussed here for the Phase III steady-state and Phase IV coupled models represent the end of the simulation sequence based on the statistical-uncertainty-propagation methodology. In terms of the IAEA CRP on HTGR UAM, no other results have so far been published on the Phase III or Phase IV uncertainty assessments, and the three objectives listed above are thus seen as important and unique contributions of this research to the field of HTGR core simulation.

The layout of this chapter is similar in structure to Chapters 6 and 7. The specifications for the coupled steady-state Exercise III-1 are reviewed in Section 8.1.1, followed by an overview of the simulation methodology chosen for this work in Section 8.1.2. The uncertainty and sensitivity results obtained for the P/R MHTGR-350 steady-state exercises are discussed in Section 8.1.3 and 8.1.4, respectively; finally, the steady-state discussion is concluded in Section 8.1.5. The coupled transient uncertainty and sensitivity results obtained for the CRW event are presented in Section 8.2.2 and 8.2.3, respectively.

## 8.1 MHTGR-350 Exercise III-1: Coupled Core Steady-State

### 8.1.1 Specification of the IAEA CRP on HTGR UAM Coupled Core Steady-State Cases

The current draft IAEA CRP on HTGR UAM specifications (Strydom 2018) defines Exercise III-1 as a steady-state core calculation focused on the HFP neutronics and thermal-hydraulics parameters. Input uncertainties used in the Chapter 4 and 5 stand-alone cases (Ex. II-2 and II-4) are combined in a coupled model, and the main FOMs are the eigenvalue and the maximum power and fuel-temperature values. The draft specifications do not specify if a model with bypass flows should be used (because not all participants might have this capability), but due to space limitations, only the results generated with the RELAP5-3D model that includes 11% bypass flows are included in this work.

### 8.1.2 Modeling Approach for the Coupled Steady-State Uncertainty and Sensitivity Assessment

The Exercise III-1 steady-state P/R model is a combination of the mixed-core PHISICS model developed for Exercise II-2b and the Exercise II-4 RELAP5-3D model presented in Chapter 7. The main attributes of the coupled model are summarized below.

- The fixed 1,200 K isothermal-temperature restriction used for the Exercise II-2b RELAP5-3D model is replaced with the standard coupled iterative scheme that allows the power and temperature fields to converge to a steady-state solution as a function of time.
- The Exercise III-1 model is identical to the P/R model developed for the OECD/NEA MHTGR-350 benchmark Exercise I-2b—i.e. 11% bypass flow and constant material properties as described in Section 7.2. Only the results obtained for the rodged Mixed Core 2ab\_rR are reported here because it has been shown in Section 6.2.3 that the addition of the peripheral Cell I (i.e. using core 2ab\_lrR) did not result in significant changes to uncertainty and sensitivity parameters.
- The original location of the control-rod bank for the MHTGR-350 EOL core was specified to be at the bottom of the first fuel block (79 cm into the active core). During development of the specifications for the CRW transient (Exercise IV-2); however, it was found that this location is too shallow to produce the desired reactivity addition of at least 0.5%  $\Delta k/k$  when the rods are withdrawn from this low-excess-reactivity core. The rods were therefore inserted four blocks deeper, into the bottom of the fifth fuel block (395 cm into the active core) to achieve a rod worth of approximately 0.6%  $\Delta k/k$ .

CHAPTER 8: MHTGR EXERCISE III 1 AND IV 2: COUPLED CORE NEUTRONICS AND THERMAL FLUIDS STEADY-STATE AND CRW TRANSIENT

- It was shown in Section 4.2 that the use of eight or 26 energy groups led to significant differences in the best-estimate/nominal results, but also that the 8-group uncertainty and sensitivity data were very similar to the 26-group data. Due to the computational expense of performing coupled transients in 26 groups, the investigation in this chapter is limited to comparisons of the 8-group U/SA data with a 2-group energy structure (one fast and one thermal group). The objective is to assess whether a 2-group steady-state model can still produce acceptable *uncertainty* results, even if it is well-known that *best-estimate* HTGR core simulation accuracy is not acceptable using only two energy groups (see Section 2.2.2).

As indicated in Section 6.1, the perturbed Phase I NEWT cross-section library files generated with SCALE/Sampler can be used in various sequences for the Phase II core exercises. In this chapter, the U/SA results for three variants of the coupled steady-state Exercise III-1 are discussed. The current draft Phase III benchmark specification lists only a single case, combining the effects of both uncertainties in neutronics and thermal fluid input parameters, but as shown in Figure 8-1, three permutations of the coupled steady-state are actually possible:

- *Exercise III-1a:* The nominal RELAP5-3D model provides temperature feedback to 1,000 perturbed PHISICS models to obtain 1,000 unique converged steady-state solutions. This sequence isolates the impacts of cross-section uncertainties.
- *Exercise III-1b:* The nominal PHISICS model (using unperturbed cross-sections) provides neutronics feedback to 1,000 perturbed RELAP5-3D models to obtain another unique set of 1,000 converged steady-state solutions. This sequence isolates the impacts of thermal fluid uncertainties.
- *Exercise III-1c:* The perturbed RELAP5-3D and PHISICS models are combined randomly to obtain a third unique set of 1,000 steady-states. This sequence combines the impacts of both cross-section and thermal fluid uncertainties.

The results obtained for all three options are discussed in this chapter, but the main focus is on Exercise III-1c, which represents one of the main contributions of this work because it completes the propagation of cross-section uncertainties from the Phase I lattice models to the Phase III coupled steady-state models. Limited comparisons are also made with the results obtained for the 1,200 K isothermal cores discussed in Chapter 5 to assess the changes caused by temperature feedback from the RELAP5 3D model. In addition to the three Exercise III-1 options, Figure 8-1 shows the differences between the Phase II and Phase III cases, and how the models developed for Phase II are linked to the Phase III exercises.

## CHAPTER 8: MHTGR EXERCISE III 1 AND IV 2: COUPLED CORE NEUTRONICS AND THERMAL FLUIDS STEADY-STATE AND CRW TRANSIENT

The temperature dependencies of the cross-section libraries are also shown in Figure 8-1. Exercise II-2 used 1,000 perturbed cross-section sets for each of the composite lattice cells—2a, 2b, r and R (see Section 6.2.2). Because no temperature feedback was required, these 4,000 microscopic ft30f001 AMPX libraries could be generated for a single temperature point (1,200 K).

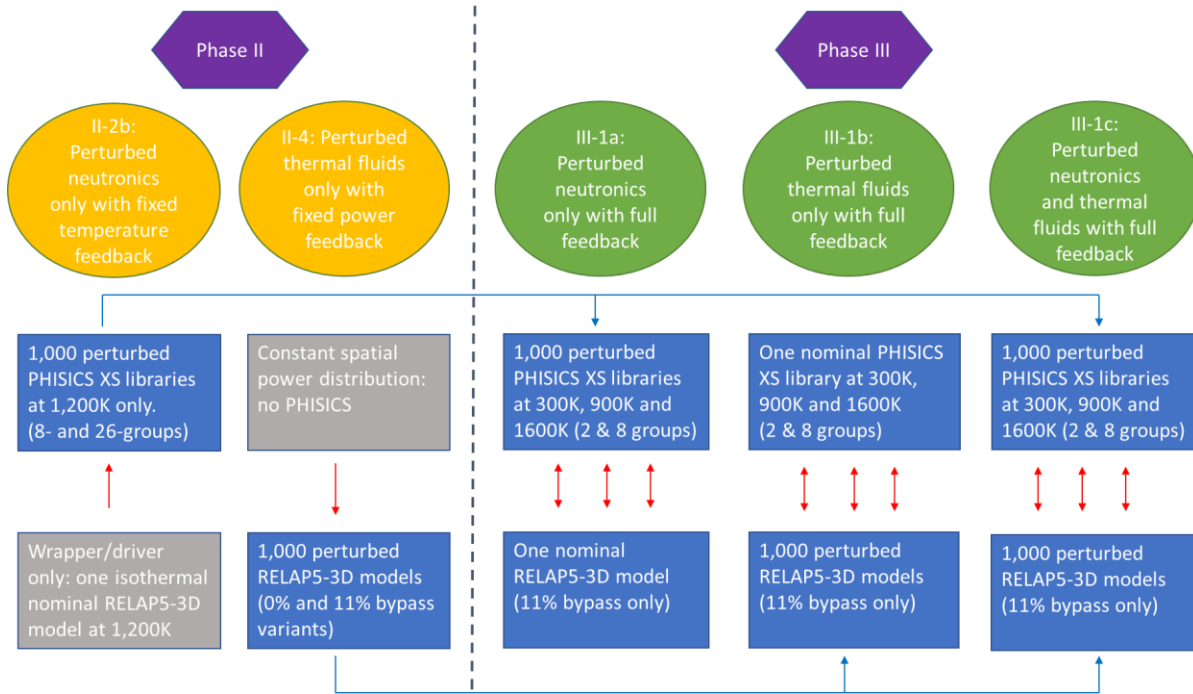


Figure 8-1. Exercise III-1 PHISICS and RELAP5-3D permutations<sup>46</sup>.

For the coupled feedback between PHISICS and RELAP5-3D, however, the cross-sections must be tabulated as functions of the fuel, moderator and reflector feedback temperatures ( $T_f$ ,  $T_m$  and  $T_{refl}$ )<sup>47</sup>. A minimum of three temperature points is usually required to capture the variances of the cross-sections over the expected temperature range because PHISICS will perform the cross-section construction based on an interpolation between the two closest points. In total, 72,000 NEWT lattice calculations<sup>48</sup> were performed at 300 K, 900 K and 1,600 K for the rodged mixed core using the four lattice models for the fresh and depleted fuel and rodged/unrodged reflector blocks.

<sup>46</sup> In this figure, the shorthand notation “XS” is used for cross-section for a more compact representation.

<sup>47</sup> PHISICS allows the tabulations of cross-sections against either the temperatures or the square root of the temperatures. Both approaches were tested, and almost identical results were obtained for a subset of the core cases. The direct temperature-tabulation method was implemented for all subsequent calculations.

<sup>48</sup> One thousand perturbed NEWT lattice cells are required for each of the four models (i.e., 2a, 2b, r and R) and three temperature points. With  $T_f = 300K$  and  $T_m = 300K$  written as 300\_300, a total of 9,000 AMPX libraries are generated per unit cell for the permutations 300\_300, 300\_900, 300\_1600, 900\_300, 900\_900, etc. In total  $9,000 \times (2a, 2b, r, R) \times (2g, 8g) = 72,000$  NEWT 252-g lattice calculations were therefore required.

## CHAPTER 8: MHTGR EXERCISE III 1 AND IV 2: COUPLED CORE NEUTRONICS AND THERMAL FLUIDS STEADY-STATE AND CRW TRANSIENT

Finally, it should be noted that Exercise III-1c actually consists of 1,000,000 possible permutations: perturbed PHISICS Model 1 can be coupled to perturbed RELAP5-3D Model 1, or any of the other 999 available perturbed RELAP5-3D models. A single set of 1,000 samples is therefore only one example<sup>49</sup> of a much-larger probability space.

Future research could include the construction of a reduced-order model (ROM) that would preserve the characteristics of this large total probability space, without calculating all possible permutations. For example, Alfonsi et al (2018) used RAVEN to construct a ROM of HTGR decay heat models that allow many perturbed SCALE/ORIGEN parameters to be considered. The computational effort to create such a ROM is beyond the scope of the current work.

### 8.1.3 Exercise III-1 Uncertainty Results

A summary of the P/R sample eigenvalue ( $k_{\text{eff}}$ ), AO, PP, control-rod worth, and MFT means and standard deviations ( $\sigma$ ) obtained for the Exercise III-1a 2-and 8-group core models are presented in Table 8-1. *Only cross-section perturbations were considered for the model variants shown here.* The rodged and unrodged Exercise II-2 results at constant 1,200 K temperatures (1200\_xxx) that were discussed in Section 6.2.2 are included in this table for comparison with the metrics obtained for the coupled P/R Exercise III-1 models. The  $\sigma$  values are shown in relative units (i.e., to the mean in %).

Table 8-1. P/R mean and  $\sigma$  values for the III-1a 2- and 8-group core models (sets of 1,000 each).

| Parameter      | 2-group                             |               |         |          |         |         | 8-group |          |
|----------------|-------------------------------------|---------------|---------|----------|---------|---------|---------|----------|
|                | 1200_2a_2b_r                        | 1200_2a_2b_rR | 2a_2b_r | 2a_2b_rR | 2a_r    | 2a_rR   | 2a_2b_r | 2a_2b_rR |
|                | Eigenvalue ( $k_{\text{eff}}$ )     |               |         |          |         |         |         |          |
| mean ( $\mu$ ) | 1.00989                             | 1.00337       | 1.02355 | 1.01720  | 1.06048 | 1.05380 | 1.03783 | 1.03203  |
| $\sigma$ (%)   | 0.447                               | 0.447         | 0.442   | 0.442    | 0.492   | 0.492   | 0.445   | 0.445    |
|                | PP                                  |               |         |          |         |         |         |          |
| Mean           | 1.340                               | 1.696         | 1.971   | 1.553    | 1.937   | 1.520   | 2.042   | 1.632    |
| $\sigma$ (%)   | 0.069                               | 0.344         | 0.308   | 0.770    | 0.257   | 0.454   | 0.340   | 0.513    |
|                | AO                                  |               |         |          |         |         |         |          |
| Mean           | -0.022                              | 0.396         | -0.514  | -0.331   | -0.501  | -0.314  | -0.527  | -0.349   |
| $\sigma$ (%)   | 4.813                               | 0.778         | 0.516   | 2.038    | 0.440   | 1.337   | 0.489   | 1.265    |
|                | Control-Rod Worth (% $\Delta k/k$ ) |               |         |          |         |         |         |          |
| Mean           | 0.646                               |               | 0.620   |          | 0.630   |         | 0.559   |          |
| $\sigma$ (%)   | 1.385                               |               | 1.412   |          | 1.421   |         | 1.286   |          |
|                | Maximum Fuel Temperature (K)        |               |         |          |         |         |         |          |
| Mean           | 1200                                | 1200          | 1123    | 1175     | 1102    | 1174    | 1146    | 1199     |
| $\sigma$ (%)   | 0.0                                 | 0.0           | 0.071   | 0.072    | 0.086   | 0.056   | 0.056   | 0.086    |

<sup>49</sup> In general uncertainty quantification literature, these examples of combined models are called “realizations”.

### ***Eigenvalue***

The core  $k_{\text{eff}}$  mean values vary significantly (~4%) between the mixed (2a-2b-r) and fresh cores (2a-r), but the main observation from Table 8-1 is that, in contrast to these large  $k_{\text{eff}}$  differences, the  $\sigma$  only vary between 0.44 and 0.49%. This is a relatively tight uncertainty band for cores containing different fuel-loading patterns and rodded and unrodded reflector blocks. The uncertainties caused in the eigenvalue by cross-section data uncertainties are, therefore, mostly insensitive to the spectral environment (e.g. if the rodded and unrodded core  $\sigma$  are compared), which is consistent with the observations made in Section 4.2.2 as well.

### ***Power Peaking***

The two isothermal mixed cores (1200\_2a\_2b\_r/R) are much less reactive due to the relatively high uniform temperature (1,200 K) of the fuel and graphite in the core region. For the MHTGR-350 core with temperature feedback, it is shown in Figure 8-2 that the upper regions of inner FR1 are much colder due to the 350°C inlet-gas temperature at the top of the core. This temperature difference between the isothermal core and the cores with temperature feedback also results in very different axial-power distributions, as shown in Figure 8-3 for FR3. The unrodded isothermal core has an almost perfect cosine power profile, and the effect of the control-rod insertion can clearly be seen in the downward movement of the power peak (shown as a blue dotted line). In contrast to this, the mixed cores that include thermal feedback display much more top-peaked power profiles due to the colder fuel and moderator temperatures in the upper regions of the core. The change in axial profiles between the rodded and unrodded cores with feedback are also much less significant than the isothermal cores the temperature effect the spatial power production.

For cores with thermal feedback, unrodded cores produced the highest mean PP values due to the shift in power generation in the upper regions of the core. The effect of control-rod insertion can best be seen in this parameter: both the fresh and mixed rodded cores have significantly lower PP values than the unrodded core equivalents. It can be seen in Table 8-1 that the 2- and 8-group PP values are reasonably close to each other (i.e., within 4%), and that the 2-group models seem to underestimate the core PP slightly. This could be expected from the approximations made with only one fast- and one thermal-energy group used in the INSTANT transport solution (e.g., in the two-group formulation the thermal upscattering in the thermal region is not included and resonance absorption by  $^{238}\text{U}$  and  $^{239}\text{Pu}$  is not accurately determined, compared to eight or more groups).

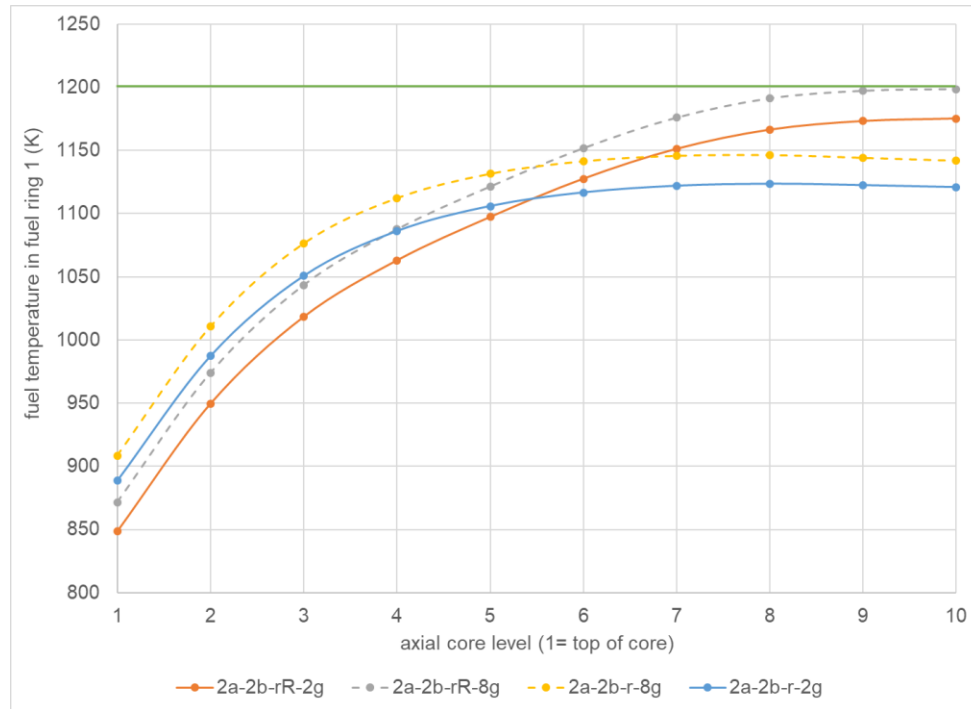


Figure 8-2. Comparison of FR1 temperature (K) axial profiles for the 2-g and 8-g core models with the 1,200 K isothermal 8-group model profile.

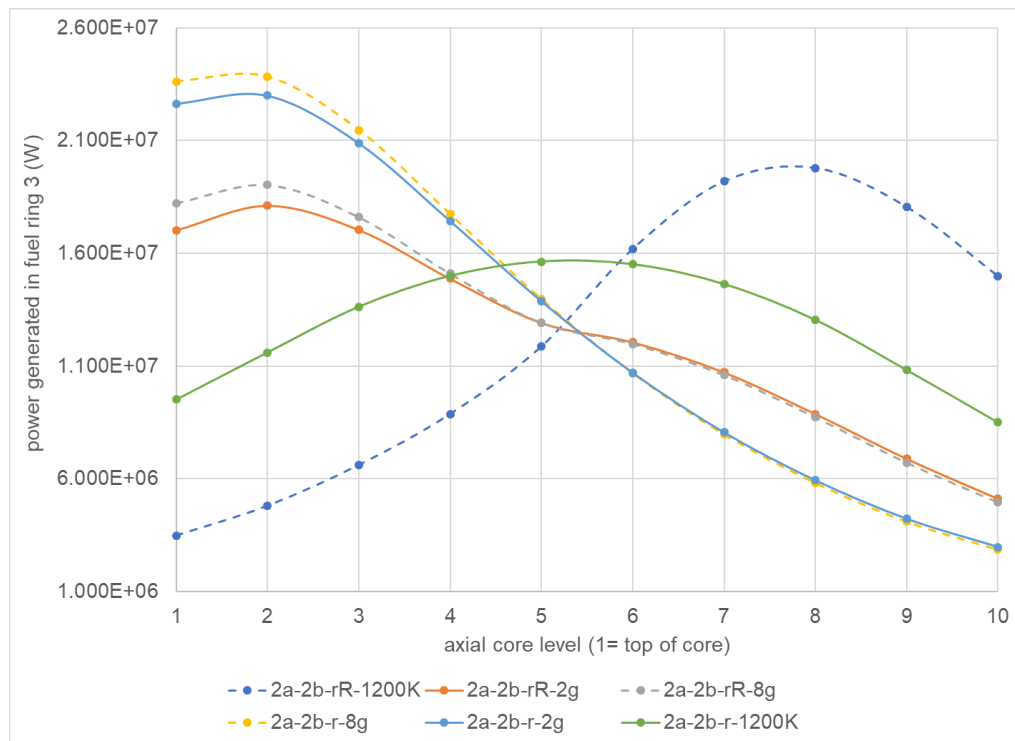


Figure 8-3. Comparison of FR3 axial power (W) axial profiles for the 2-g and 8-g core models with the rodDED and unroDDed isothermal 8-group model profiles.

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Similar to the observations made in Section 4.2.2, the PP  $\sigma$  values follow an inverse trend to the mean PP values: the perturbed rodded cores produced higher  $\sigma$  values than the unrodded cores. The PPs  $\sigma$  of the mixed cores vary between 0.31 and 0.51%, while the fresh-core values are slightly lower. The uncertainties in the cross-section data resulted, therefore, in significant changes to the PP values for the core models that included temperature feedback. The almost-cosine axial-power shape of the unrodded isothermal core resulted in a very small PP  $\sigma$  (0.07%).

### ***Axial Offset and Control-Rod Worth***

Of the FOMs included in this section, the AO shows the highest  $\sigma$  values, ranging between 0.44 and 2.04% for the cores that included thermal feedback (Table 8-1). In general, the trends are the same as discussed for the PP parameter, with  $\sigma$  the largest for the smallest mean values in an inverse relationship. By subtracting the rodded and unrodded cases, control-rod worth values can also be calculated. The rod worth is defined here as the worth of the rods when fully withdrawn from the bottom of the fifth fuel block (e.g. 79 cm x 5 = 395 cm inserted). The control-rod worths shown in Table 8-1 are relatively close for all three core types (i.e. mixed isothermal, mixed, and fresh cores with thermal feedback), ranging from 0.56% for the 8-group mixed core to 0.65% for the isothermal 8-group mixed core. The control-rod worth  $\sigma$  values are again similar between these core models, and significant enough (1.29-1.42%) to be of interest to core designers to consider for operational and shutdown rod margin characterization.

### ***Maximum Fuel Temperature<sup>50</sup>***

The MFT is an important safety-case FOM. In the case of HTGRs, it is unfortunately not easy (or even possible at all) to measure this parameter, but it can nevertheless be calculated and is commonly used as a proxy for failure-induced fission product release from the fuel. Thus, the impact of cross-section uncertainties on this FOM is of interest to the HTGR core design community. In the context of the current RELAP5-3D model, MFT does not mean the UCO kernel temperature in the center of a fuel compact, but rather the maximum value of the 30-ring-homogenized fuel temperatures in the three fuel rings (see Appendix B-1 for more detail).

It is shown in Table 8-1 that although the mean MFT varies by up to 96 K between these models (~9%), the  $\sigma$  values of these sample populations are all very similar and small (<0.1%, or 2 K). However, this observation is strictly only valid for the one spatial location where the MFT occurs (at the bottom of FR1). It is shown in the discussion of spatial results later in this section that higher uncertainties, up to 0.25%, are obtained in the cooler regions of the core.

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<sup>50</sup> The MFT is defined in Section 6.2.1 and Appendix B-1 as the maximum value of the 30 ring-homogenized fuel temperatures for the three fuel rings on the ten axial levels.

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This is not seen as a significant impact because a difference of 0.25% on 900 K (or 2.25 K) would not impact margin calculations at all and are well within most coupled modeling uncertainties.

In conclusion, it is therefore observed that, although the power distribution and control-rod worths are affected more significantly by cross-section uncertainties, the impact of these variations on the fuel temperatures is insignificant.

A comparison of the mean and  $\sigma$  values obtained for Exercises III-1a, III-1b, and III-1c is shown in Table 8-2. The designation “2g\_XS” refers to the perturbation of cross-sections only, and all results are obtained for sets of 1,000 fully converged coupled steady-state P/R models.

Table 8-2. P/R mean and  $\sigma$  values for the 2- and 8-group Exercise III-1a, III-1b and III-1c core models (sets of 1,000 each).

| Metric/Case                  | Exercise III-1a     |         | Exercise III-1b | Exercise III-1c |          |
|------------------------------|---------------------|---------|-----------------|-----------------|----------|
|                              | 2g_XS <sup>51</sup> | 8g_XS   | 2g_TF           | 2g_XS_TF        | 8g_XS_TF |
| Eigenvalue ( $k_{eff}$ )     |                     |         |                 |                 |          |
| Mean ( $\mu$ )               | 1.01720             | 1.03203 | 0.99225         | 0.99236         | 1.00671  |
| $\sigma$ (%)                 | 0.445               | 0.445   | 0.161           | 0.469           | 0.463    |
| Axial Offset (AO)            |                     |         |                 |                 |          |
| Mean ( $\mu$ )               | -0.33               | -0.35   | -0.33           | -0.33           | -0.35    |
| $\sigma$ (%)                 | -2.04               | -1.26   | -2.69           | -2.92           | -1.86    |
| Power Peaking (PP)           |                     |         |                 |                 |          |
| Mean ( $\mu$ )               | 1.55                | 1.63    | 1.55            | 1.55            | 1.63     |
| $\sigma$ (%)                 | 0.77                | 0.51    | 1.07            | 1.18            | 0.69     |
| Maximum fuel temperature (K) |                     |         |                 |                 |          |
| Mean ( $\mu$ )               | 1174                | 1198    | 1175            | 1175            | 1198     |
| $\sigma$ (%)                 | 0.05                | 0.09    | 1.45            | 1.45            | 1.54     |

The eigenvalue  $\sigma$  values for the 2- and 8-group cross-section and combined cross-section and thermal fluid models are very similar (0.45–0.47%), but the 2-group thermal fluid model produced a significantly lower eigenvalue standard deviation (0.16%). The 2-group thermal fluid mean eigenvalue is therefore not impacted to the same degree when compared to the inclusion of cross-sections perturbations, and aspect that is further explored in the sensitivity assessment Section 8.1.4. This can also be seen from the much-smaller sample population range (defined as  $[k_{eff\_max}-k_{eff\_min}]$  out of the 1,000 steady-states) for the 2g\_TF model (1,208 pcm), compared to the other four model ranges (2,989–3,024 pcm). In contrast to this observation, the standard deviations of the other 2g\_TF FOMs are mostly similar to the other perturbed models.

<sup>51</sup> XS\_2g and XS\_8g in Table 8-2 corresponds to 2a\_2b\_rR\_2g and 2a\_2b\_rR\_8g in Table 8-1.

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In general, the AO produced the largest standard deviations (1.3–2.9%), followed by the MFT (0.1–1.5%) and the PP (0.7–1.2%). The differences between the various steady-state models are the largest for the MFT, where the impact of thermal fluid uncertainties can clearly be observed. The MFT standard deviations of both cross-section (XS)-only models are much lower (<0.1%) than the models that include thermal fluid perturbations, where standard deviations of up to 1.54% (18 K) are calculated.

The eigenvalue standard deviations therefore seem to be particularly sensitive to one or more of the perturbed cross-section reactions, while the MFT is mostly sensitive to perturbed thermal fluid parameters. The 2-group models tend to overestimate AO and PP population standard deviations when compared to the 8-group values; a trend also identified in Section 8.1.4. The 2-group models do, however, perform relatively well when used to assess the impacts on the eigenvalue and MFT FOMs, where standard-deviation differences with the 8-group results are insignificant.

### **Spatial Power Data**

Integral parameters like the eigenvalue or AO are useful indicators of trends during the initial comparison phase, but the impact of cross-section and thermal fluid input uncertainties ultimately need to be assessed for local reaction rates, fluxes, and power densities. Examples of the mean and standard deviation fuel temperature distributions in the three fuel rings are provided in Table 8-3 and Table 8-4. Only the 2-group data is included in these tables for clarity; the full data set can be found in Appendix D-1 Table D-1 (Exercise III-1a fuel temperature), Table D-2 (Exercise III-1a power), Table D-3 (Exercise III-1c fuel temperature) and Table D-4 (Exercise III-1c power).

It can be seen in Table 8-3 that the mean fuel temperatures for the various 2-group models are very similar at every location<sup>52</sup>, but some significant spatial variances are observed between the models' standard deviations in Table 8-4. The information in these two tables is also presented in Figure 8-4 for FR1.

The fuel-temperature standard deviations for the Exercise III-1a (XS-only perturbations) are consistently significantly smaller than the standard deviation for the Exercise III-1b and III-1c models, indicating that the perturbation of cross-sections had a smaller impact on the fuel temperature as the perturbation of thermal fluid input parameters. In relative % units, the standard deviations for the Exercise III-1a model peak in the upper core regions at 0.25%, in contrast to standard deviations increasing towards the bottom of the core for the other two models to a peak value of 1.45%. This effect is even more pronounced in absolute (K) units because the fuel temperature increases by almost 350 K towards the core exit.

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<sup>52</sup> If it is assumed that the fuel temperature could be characterized as a normal distribution, it should be expected that the mean of a large number of random samples would approach the nominal value of the distribution.

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The perturbations in the thermal fluid parameters had significant impact on fuel temperatures (up to 1.45% or 18 K), but the addition of cross-section perturbations did not change this dominant impact at all (e.g., if the two bold values in Table 8-4 for FR1 are compared Exercise III-1b and III-1c).

Table 8-3. Mean fuel temperature (K) distribution for Exercises III-1a, III-1b and III-1c.

| Axial level | 2g_XS (Exercise III-1a) |      |     | 2g_TF (Exercise III-1b) |      |     | 2g_XS_TF (Exercise III-1c) |      |     |
|-------------|-------------------------|------|-----|-------------------------|------|-----|----------------------------|------|-----|
|             | FR1                     | FR2  | FR3 | FR1                     | FR2  | FR3 | FR1                        | FR2  | FR3 |
| 1           | 849                     | 751  | 729 | 848                     | 751  | 728 | 848                        | 751  | 728 |
| 2           | 951                     | 819  | 798 | 950                     | 818  | 798 | 950                        | 818  | 798 |
| 3           | 1020                    | 868  | 847 | 1018                    | 867  | 846 | 1018                       | 867  | 846 |
| 4           | 1064                    | 900  | 881 | 1063                    | 899  | 880 | 1063                       | 899  | 880 |
| 5           | 1098                    | 927  | 910 | 1098                    | 926  | 909 | 1097                       | 926  | 909 |
| 6           | 1128                    | 953  | 943 | 1128                    | 953  | 942 | 1128                       | 953  | 942 |
| 7           | 1151                    | 975  | 968 | 1152                    | 975  | 967 | 1152                       | 975  | 967 |
| 8           | 1166                    | 989  | 983 | 1167                    | 989  | 982 | 1167                       | 989  | 983 |
| 9           | 1173                    | 996  | 991 | 1174                    | 996  | 990 | 1174                       | 996  | 990 |
| 10          | 1174                    | 1001 | 993 | 1175                    | 1001 | 993 | 1175                       | 1001 | 993 |

Table 8-4. Fuel temperature  $\sigma$  (%) distribution for Exercises III-1a, III-1b and III-1c.

| Axial level | 2g_XS (Exercise III-1a) |      |      | 2g_TF (Exercise III-1b) |      |      | 2g_XS_TF (Exercise III-1c) |      |      |
|-------------|-------------------------|------|------|-------------------------|------|------|----------------------------|------|------|
|             | FR1                     | FR2  | FR3  | FR1                     | FR2  | FR3  | FR1                        | FR2  | FR3  |
| 1           | 0.25                    | 0.22 | 0.19 | 1.34                    | 1.19 | 1.10 | 1.37                       | 1.21 | 1.12 |
| 2           | 0.24                    | 0.24 | 0.18 | 1.40                    | 1.24 | 1.16 | 1.42                       | 1.26 | 1.18 |
| 3           | 0.20                    | 0.22 | 0.15 | 1.37                    | 1.24 | 1.16 | 1.38                       | 1.26 | 1.18 |
| 4           | 0.16                    | 0.19 | 0.11 | 1.32                    | 1.22 | 1.14 | 1.33                       | 1.22 | 1.15 |
| 5           | 0.12                    | 0.15 | 0.07 | 1.29                    | 1.20 | 1.13 | 1.29                       | 1.20 | 1.13 |
| 6           | 0.09                    | 0.12 | 0.03 | 1.29                    | 1.22 | 1.14 | 1.29                       | 1.21 | 1.14 |
| 7           | 0.07                    | 0.09 | 0.05 | 1.34                    | 1.26 | 1.17 | 1.33                       | 1.25 | 1.17 |
| 8           | 0.07                    | 0.07 | 0.07 | 1.40                    | 1.30 | 1.20 | 1.39                       | 1.30 | 1.20 |
| 9           | 0.07                    | 0.05 | 0.10 | 1.44                    | 1.34 | 1.22 | 1.43                       | 1.33 | 1.23 |
| 10          | 0.07                    | 0.04 | 0.13 | <b>1.45</b>             | 1.36 | 1.23 | <b>1.45</b>                | 1.35 | 1.24 |

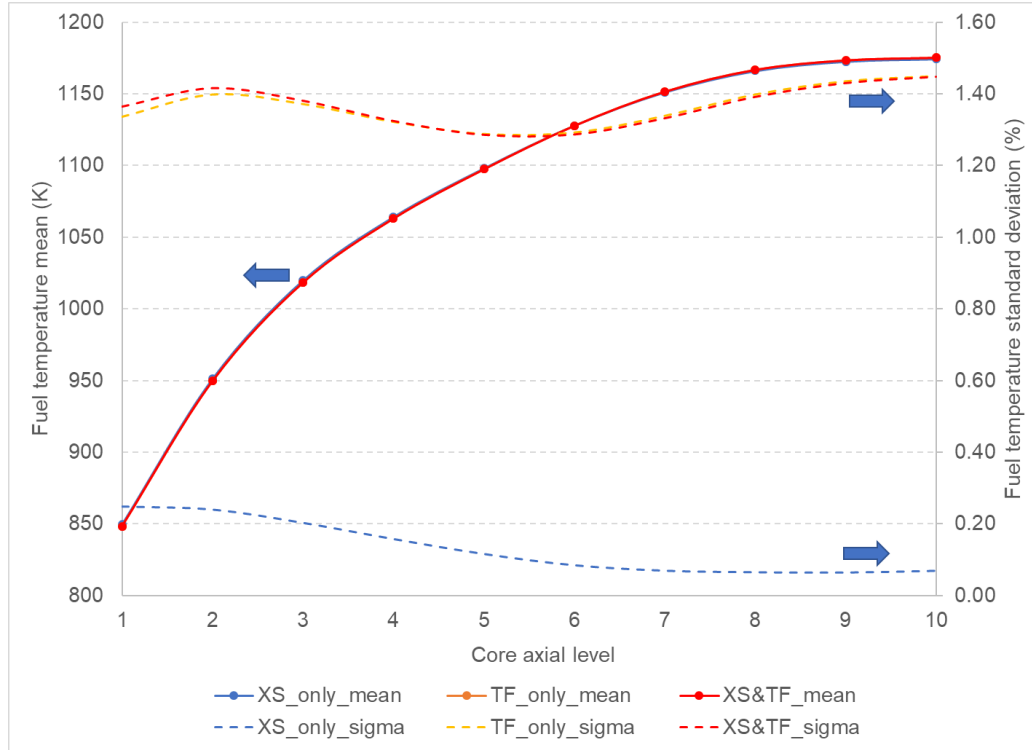


Figure 8-4. Comparison of 2-group mean (K) and standard deviation (%) fuel temperature per axial level in FR1 for Exercises III-1a, III-1b and III-1c.

The mean and standard deviation of the power generation are presented in Figure 8-5 for FR3, in which core maximum power is generated in the second axial location from the top due to neutron backscatter from the reflector (the full power distribution is shown in Appendix D, Figure D-2). The mean power distribution is again almost identical between the three Exercise III-1 models, similar to the fuel-temperature data. The axial-power generation standard deviations for Exercise III-1a are likewise smaller than the uncertainties in the Exercise III-1b and III-1c models, but all three axial distributions reach maxima in the upper and lower parts of the core. In absolute units (MW), the highest uncertainties occur in the upper region of the core where the power peak is located. The lowest relative standard deviations occur near axial level five—i.e. at the bottom of the control rods.

Cross-section perturbations seem to lead to a small increase in standard deviations in the first and final-two axial levels (i.e. if the orange and red lines are compared), but power-generation uncertainties are also dominated by thermal fluid perturbations to a large degree.

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As can be expected from the definition of local power as the normalized total reaction rate, perturbations of cross-sections did result in a 0.2–2.0% standard deviation in the local power, but the addition of thermal fluid perturbations caused significantly higher standard deviations (2.0–3.6%), especially in the upper region of the core where the peak power occurs.

These uncertainties in local power and fuel temperature are significant enough to take into account during the design-margin assessment process, but it is lower than the historic values assumed by GA of up to 15% in fuel temperatures and 10% in local power (Baxter, 2010). The value of the BEPU approach vs. very conservative assumptions is therefore illustrated by this comparison.

As final remark on the sometimes-competing impacts of coupled feedback effects, it should be noted that a decrease in the parasitic absorption neutron-capture  $^{238}\text{U}$  ( $n,\gamma$ ) cross-section (for example) would increase the local power, but since the higher power will lead to higher fuel temperature, the power would decrease during the next coupled feedback iteration. Likewise, an increase in fuel temperatures driven by thermal fluid uncertainties would decrease local power; possibly overriding competing perturbations in cross-sections.

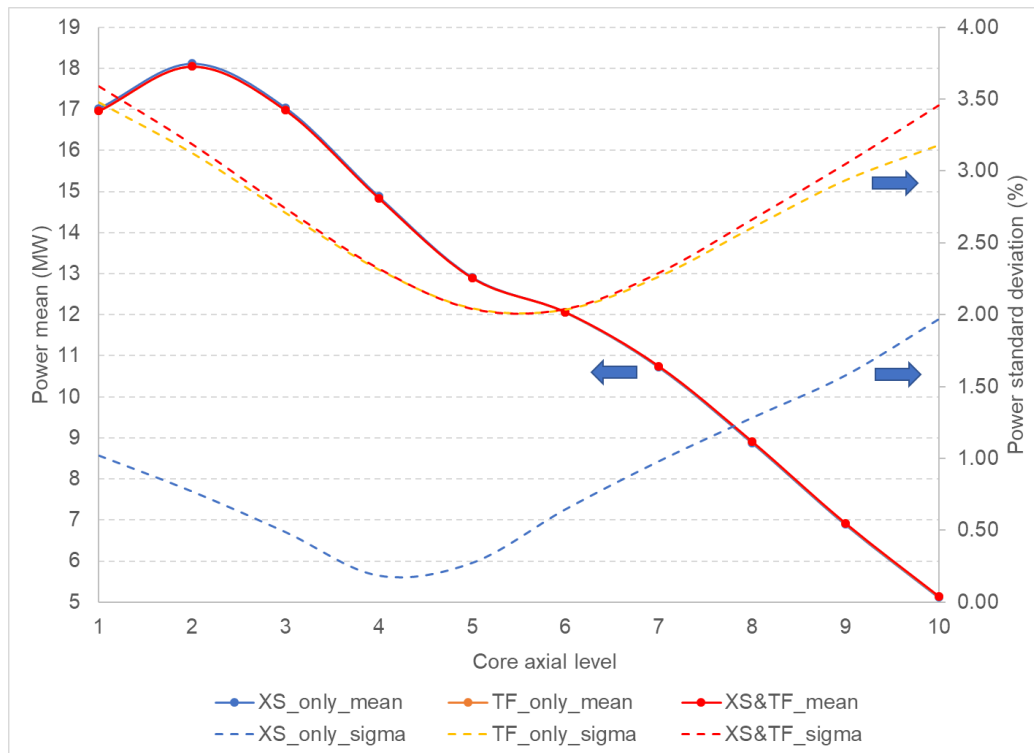


Figure 8-5. Comparison of 2-group mean (MW) and standard deviation (%) power generation per axial level in FR3 for perturbations of the cross-sections only, thermal fluids only, and both cross-sections and thermal fluids.

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The differences between the 2- and 8-group mean FR1 fuel temperatures and power generation in FR3 are shown in Figure 8-6 and Figure 8-7 respectively. The 2-group models both predict 20-25 K lower mean fuel temperatures than the 8-group models. The (user) choice of two energy groups therefore impacts the mean fuel temperatures to a slightly larger degree than the uncertainties in either cross-sections or thermal fluid input, which again illustrate the importance of selecting the proper energy group structure for best-estimate HTGR analysis.

It should however be pointed out that 25 K is still a relative small difference of less than 4%, which might be quite acceptable for scoping calculations during the early phases of design, especially if the computational cost of many calculations are factored into the cost vs. accuracy benefit analysis.

The difference between the 2- and 8-group predictions of mean power generation in the outer fuel ring is relatively small in the lower-power bottom regions of the core (Figure 8-7), but it reaches a maximum value of ~6% in the upper region of the core where the power peak is located. This difference in axial-power generation is not carried through to the fuel temperature due to the forced helium flow heat removal.

The variances in the standard deviations of the fuel temperature in FR1 and power generation in FR3 are shown in Figure 8-8 and Figure 8-9, respectively. The differences between the 2- and 8-group fuel temperatures are much smaller (<0.3%) than the differences caused by the inclusion of thermal fluid uncertainties. The power standard deviation in FR3 follows a similar trend, but since the 2- group axial-power profile is shifted downwards, differences up to 1.2% are observed in the lower regions of the core. Although the 2-group model tends to over-predict the uncertainty in the high-power upper region of the core (balanced by an underprediction in the bottom core regions), the differences between the 2- and 8-group models are probably minor enough that the 2-group approach can be used for early-stage uncertainty assessment studies. The 2-group approach is however not recommended for best-estimate steady-state analysis beyond scoping design iterations.

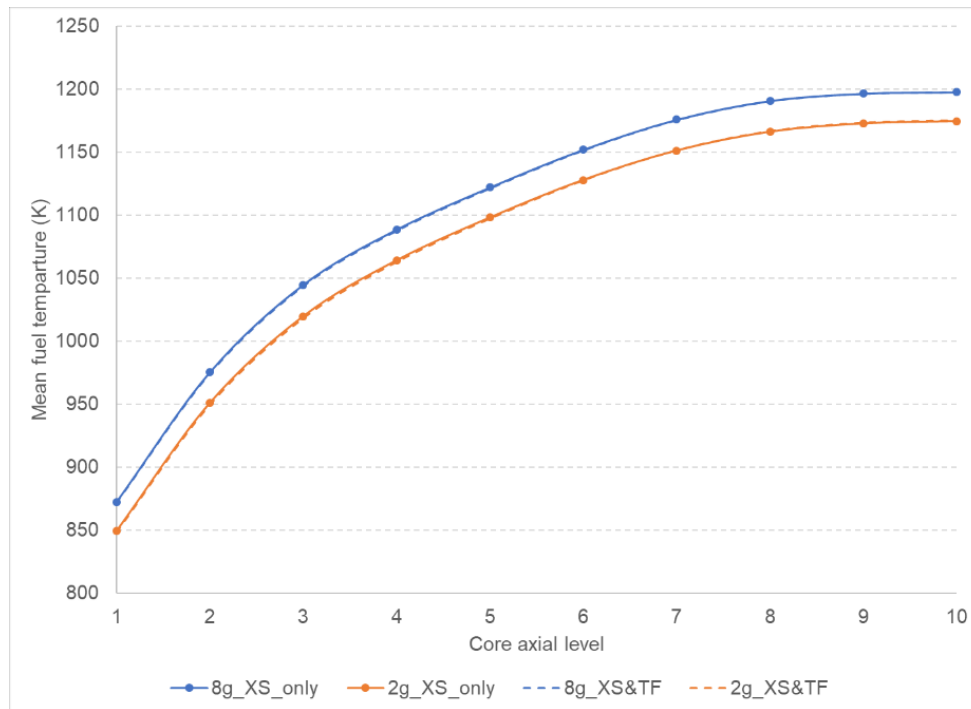


Figure 8-6. Comparison of 2- and 8-group mean fuel temperature (K) per axial level in FR1 for perturbations of the cross-sections only and both cross-sections and thermal fluids.

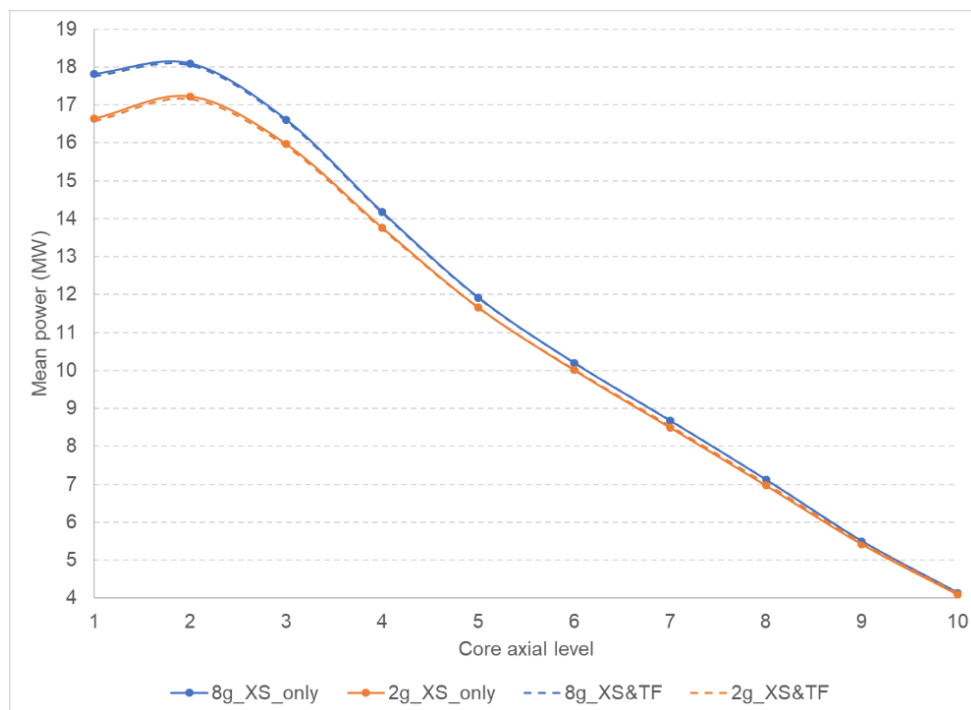


Figure 8-7. Comparison of 2- and 8-group mean power (MW) per axial level in FR3 for perturbations of the cross-sections only and both cross-sections and thermal fluids.

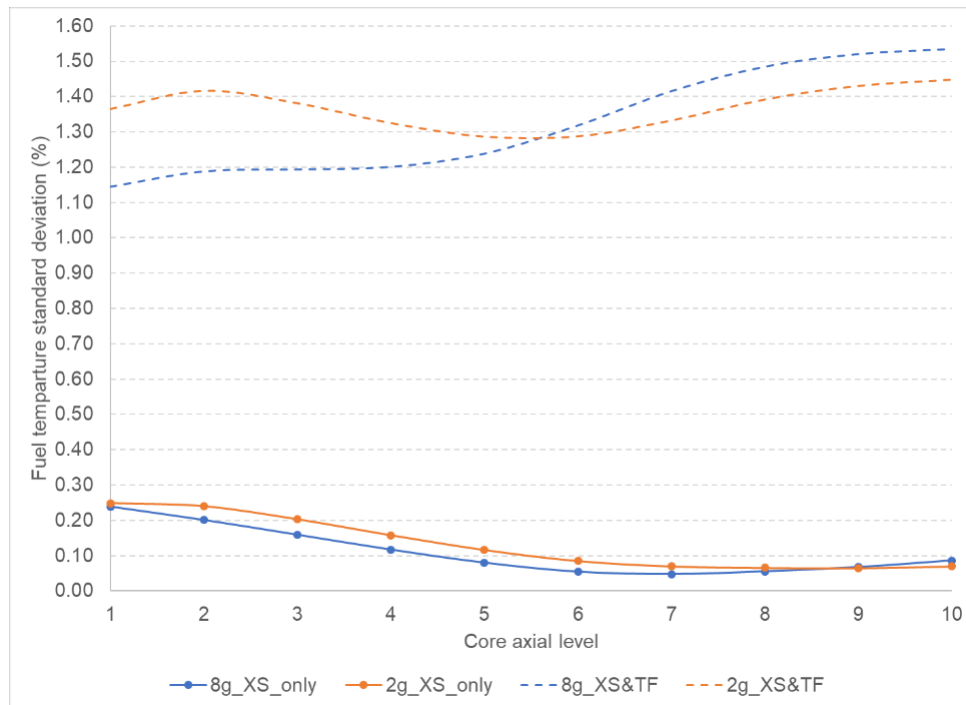


Figure 8-8. Comparison of 2- and 8-group standard deviation fuel temperature (%) per axial level in FR1 for perturbations of the cross-sections only and both cross-sections and thermal fluids.

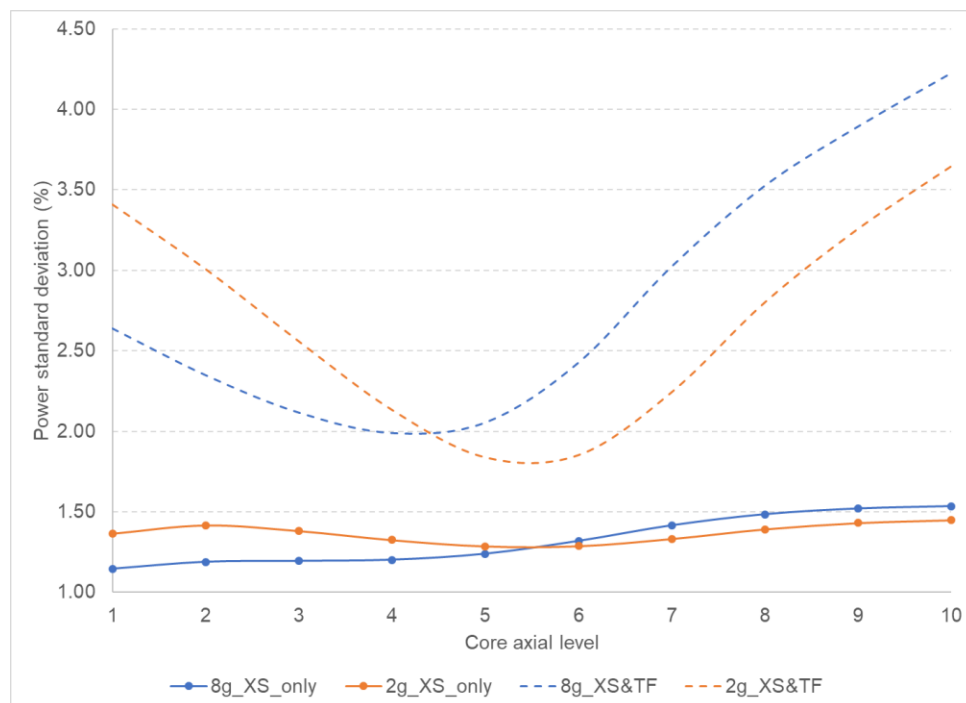


Figure 8-9. Comparison of 2- and 8-group standard deviation power (%) per axial level in FR3 for perturbations of the cross-sections only and both cross-sections and thermal fluids.

#### 8.1.4 Exercise III-1 Sensitivity Results

The two objectives of the Exercise III-1 sensitivity assessment are the identification of the major input uncertainty drivers and comparisons with the stand-alone results obtained in the previous chapters for Exercise I-2 (Section 5.2.2), Exercise II-2 (Section 6.2.3) and Exercise II-4 (Section 7.4.2). As before, RAVEN is used to calculate NSCs and PCCs, and the primary FOMs are one integral parameter ( $k_{eff}$ ) and two local spatial values (the maximum fuel temperature and maximum power). It is important to note again that RAVEN cannot be used to identify the individual contributions to the total uncertainties in the FOMs; the only available sensitivity indices are the linear regression sensitivity coefficients that represent changes in the mean FOM values for variations of 1% in the input parameter value.

Following the approach in Section 8.1.3, the sensitivity parameters are compared for the 2- and 8-group models with cross-section (XS)-only perturbed-input data, thermal fluid (TF)-only perturbed-input data, and both XS and TF perturbed-input data. The discussion is split in two sections: the first discussion is focused on the impact of TF boundary conditions and comparisons with Exercise II-4, while the second section characterizes the impact of cross-section uncertainties and comparisons with Exercise II-2.

##### ***PCCs and NSCs for thermal fluid boundary-condition uncertainties***

The PCCs and NSCs for the three FOMs and the 2g\_XS\_TF, 8g\_XS\_TF and 2g\_TF models are shown in Figure 8-10 and Figure 8-11, respectively. For clarity and comparison with the stand-alone Exercise II-4 results, only the input boundary-condition PCCs are shown here. Similar to the Exercise II-4 results discussed in Section 7.4.2, the H-451 graphite thermal conductivity and the inner-fuel-ring bypass flow is ranked fourth and fifth for Exercise III-1 as well, so the addition of neutronic feedback or cross-section perturbations did not change the relative insensitivity of the FOMs to these material-property uncertainties.

The points below summarize the major observations that can be made from the data in these two figures.

##### **2-group vs. 8-group**

- The 2- and 8-group models generally predict very similar PCCs and NSCs, but the NSCs for uncertainties in the maximum power are particularly sensitive to the number of groups utilized. This is mainly caused by the underprediction of local power densities when the 2-group formulation is used. The impact of group structure on the MFT is minimal because the convective heat transfer via forced helium flow disconnects the regions in the core where the MFT occurs (FR1 bottom block in Table D-3) and where the maximum power is generated (FR3 second block from the top in Table D-4).

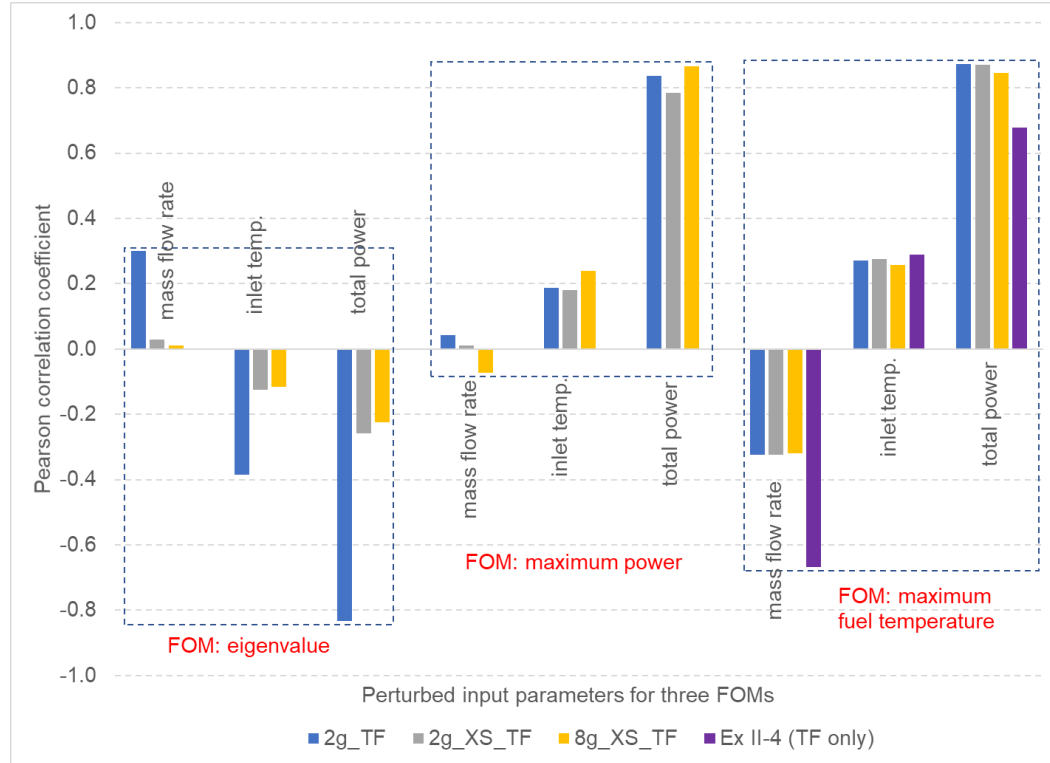


Figure 8-10. Comparison of 2- and 8-group PCCs for three FOMs and four steady-state models.

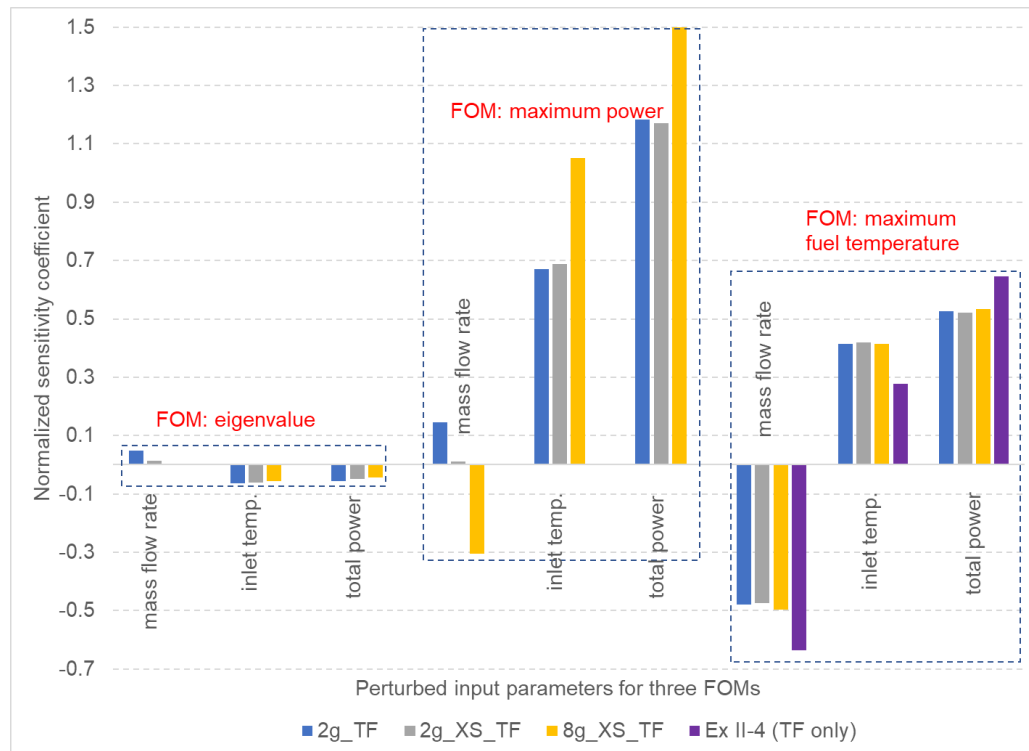


Figure 8-11. Comparison of 2- and 8-group NSCs for three FOMs and four steady-state models.

### Variances between the FOMs

- The perturbed parameters impact the uncertainties in the three FOMs in different and sometimes opposite ways: the 1% (3.5 MW) perturbation in the total power lead to increases of 0.53% (6 K) in the 8-group model mean MFT and 1.50% (0.285 MW)<sup>53</sup> in the maximum power, but a decrease of only 0.04% (40 pcm) in the eigenvalue<sup>54</sup>. As indicated in Section 8.1.3, the spatial variances across the core axial and radial dimensions are significant and can also offset each other (e.g. a rise in power in the bottom core region would increase power in the top). A spatially integrated indicator of core reactivity, such as the eigenvalue, therefore “integrates” local sensitivity and uncertainty information and could lead to inaccurate conclusions if it is not used in conjunction with other local variables.
- The ranking of the impact of the three boundary-condition input parameters also varies between the FOMs: for MFT uncertainty, the power and mass-flow rate PCCs and NSCs are almost equivalent, but for maximum power uncertainty, the mass-flow rate uncertainties are much less important than the total power uncertainties.

### Exercise II-4 stand-alone thermal fluid vs. Exercise III-1 coupled feedback

- The addition of feedback between the neutronic and TF modules decreased the NSCs for the MFT uncertainty to a small degree, but the relative ranking of the Exercise II-4 and III-1 parameters remained the same. The impact of perturbations in the mass-flow rate was larger for the stand-alone model, most likely since the power distribution remained static, compared to changes in the spatial power distribution that occurred for the coupled model with feedback.

### Thermal-fluid-only, cross-section-only, and thermal fluid and cross-section perturbations

- In general, the value and ranking of most PCCs and NSCs are very similar regardless of the perturbed-input data (TF, XS or both); e.g. perturbations of the total reactor power lead to both the largest PCC and NSC values for all FOMs and models. The first exception to this trend is the 2g\_TF PCCs for the eigenvalue, which are significantly larger than the two XS\_TF model PCCs. However, these differences are not carried through to the eigenvalue NSCs, which are all almost identical and relatively small. (This example shows the risk of depending only on one statistical indicator to identify trends).

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<sup>53</sup> The detail PCC and NSC data can be found in Table D-5 in Appendix D-1.

<sup>54</sup> See Appendix B-1 for more detail on the NSC formulation.

- The second difference occurs for the effect that uncertainties in the mass-flow rate has on maximum power uncertainty. Although the PCCs are relatively small (indicating weak linear correlation), the two 2-group NSCs are positive compared to the negative NSC for the 8-group XS\_TF models (lower mass-flow rates lead to increases in the maximum power). This is caused by the dynamics that occur in the upper core location where the peak power is generated: an increase in mass-flow rate cools the upper regions of the core down, leading to higher local-power generation. Because the 2-group models tend to underpredict local-power densities (Section 8.1.3), the 2-group model sensitivity results for this specific parameter will also contain larger uncertainties, and care should be taken with conclusions based on the 2-group model in terms of the maximum power variable. In general, a higher number of energy groups (e.g., 26-groups) would produce more accurate results, with reference results possibly obtained using 252-group or even CE Monte Carlo models if the computational expense can be afforded.

### ***PCCs and NSCs for cross-section uncertainties***

The preceding discussion focused on the impact of uncertainties in the TF input boundary conditions. To allow direct comparison with the energy-independent PCC and NSC data calculated for the other input parameters, the data in these figures (based on the detailed information in Table D-5 in Appendix D) represent the *maximum* values obtained for the 56-group energy structure, as shown in Figure D-1 in Appendix D.

The impact of cross-section uncertainties is characterized in Figure 8-12 and Figure 8-13 in terms of the 2- and 8-group PCC and NSC data, and compared with the top three TF boundary-condition parameters. The following observations can be made about the data in these two figures:

- The relative ranking of the cross-section and boundary-condition input uncertainties vary significantly between the three FOMs. In terms of both the PCC and NSC values, the eigenvalue is completely dominated by the uncertainties in the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction, followed by the  $^{239}\text{Pu}(n,\gamma)$  reaction. These two parameters have larger contributions to the eigenvalue uncertainty than any TF parameter.
- The impact of uncertainties in  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  also ranks high for the maximum fuel temperature (first for 2-groups, second for 8-groups) and the maximum power (first/second) NSCs, but the TF boundary conditions still dominates the MFT and maximum power uncertainties.

- The sensitivity of the maximum power NSCs to the energy group structure is again visible here (as is the relative insensitivity of the MFT and eigenvalue). The impact of the mass-flow rate on maximum power is likewise predicted as a positive correlation (although very weak) by the 2-group model, but much-larger differences are observed for the maximum power PCCs of the  $^{239}\text{Pu}(n,\gamma)/^{239}\text{Pu}(n,\gamma)$  and C-graphite elastic-scatter reactions: the 2-g PCC for the  $^{239}\text{Pu}(n,\gamma)/^{239}\text{Pu}(n,\gamma)$  reaction is not only much smaller than the 8-group value, but also negative. It was noted before that the selection of the thermal-cut-off energy boundary (5 eV) is not suitable to resolve the  $^{239}\text{Pu}$ -resonance region accurately, and the improvement that can be obtained with a finer 8-group structure is clearly reflected in this parameter. Not all of these PCC differences are reflected in the NSCs; e.g. the  $^{239}\text{Pu}(n,\gamma)/^{239}\text{Pu}(n,\gamma)$  NSC for the 2- and 8-group models are almost identical.

It was found in Sections 4.4.2 (VHTRC) 5.2.2 (Phase I) and 6.2.3 (Phase II) that the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction ranked in the first place in terms of its impact on the eigenvalue. For the coupled Exercise III-1 models, this reaction again produced the highest sensitivities to the eigenvalue, MFT, and maximum power uncertainties, as shown in Figure 8-14 and Figure 8-15. The results obtained with the 2- and 8-group models, where only the cross-sections were perturbed, are very similar to the simultaneous perturbation of both cross-sections and TF parameters, but only for the eigenvalue as FOM.

Perturbations in the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  and  $^{239}\text{Pu}(n,\gamma)/^{239}\text{Pu}(n,\gamma)$  reactions of the 2- and 8-group models had very different impacts on the maximum power FOM. Even if a 2-group model could be acceptable for use in scoping-level best-estimate and uncertainty assessments, the sensitivity of local parameters—such as the MFT and especially the maximum power peaking—require a higher number of energy groups that are optimized to capture the physics of the  $^{238}\text{U}(n,\gamma)$  and  $^{239}\text{Pu}(n,\gamma)$  resonance regions.

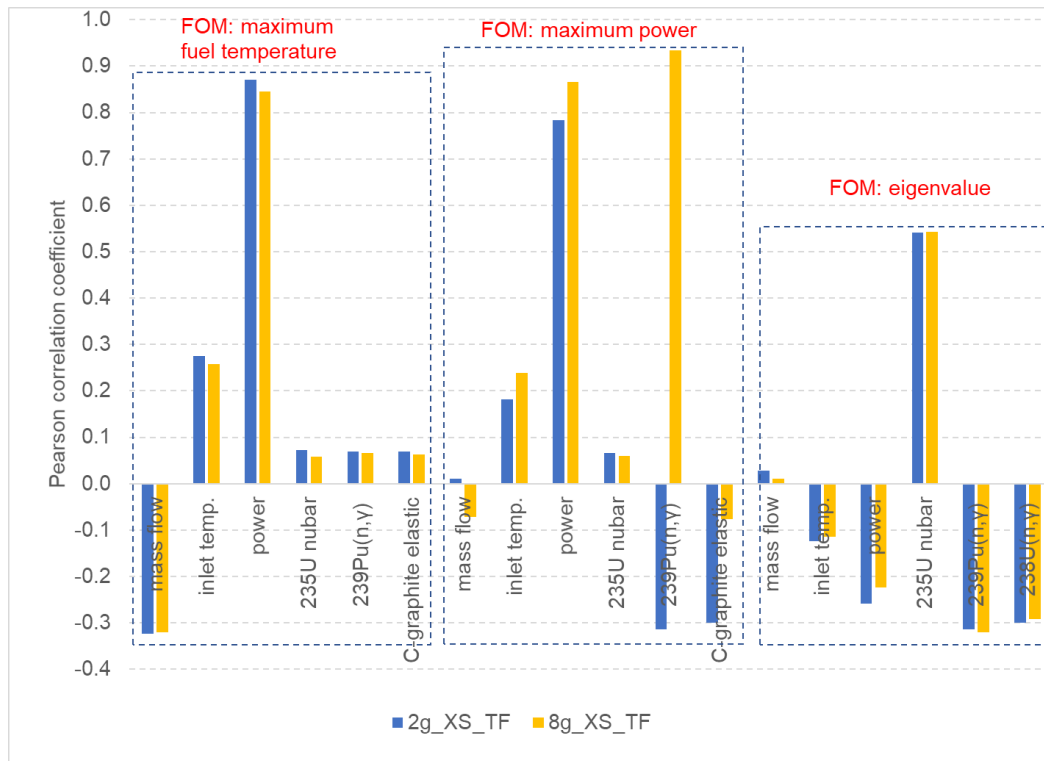


Figure 8-12. Comparison of 2- and 8-group PCCs for three FOMs and six perturbed-input parameters.

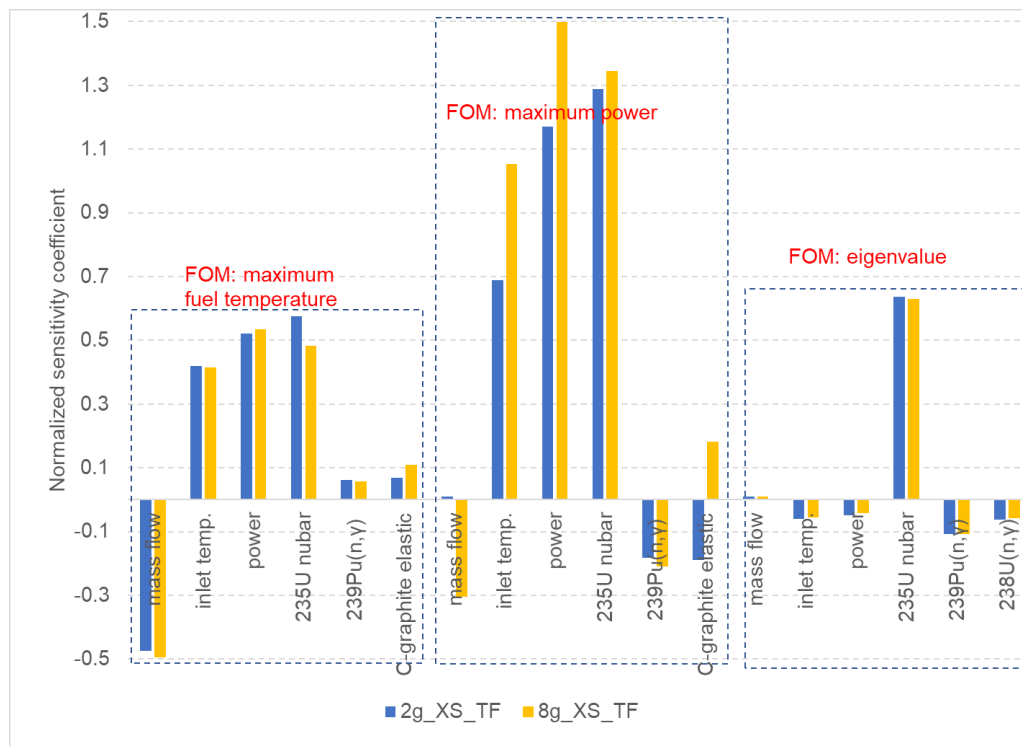


Figure 8-13. Comparison of 2- and 8-group NSCs for three FOMs and six perturbed-input parameters.

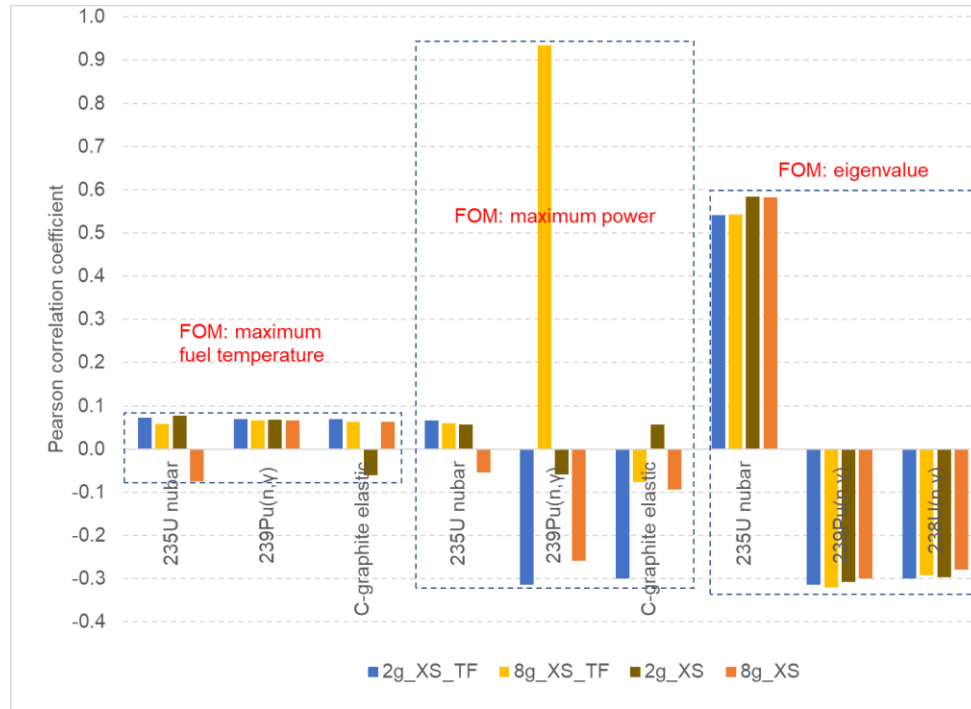


Figure 8-14. Comparison of 2- and 8-group PCCs for three FOMs and three perturbed cross-section reactions.

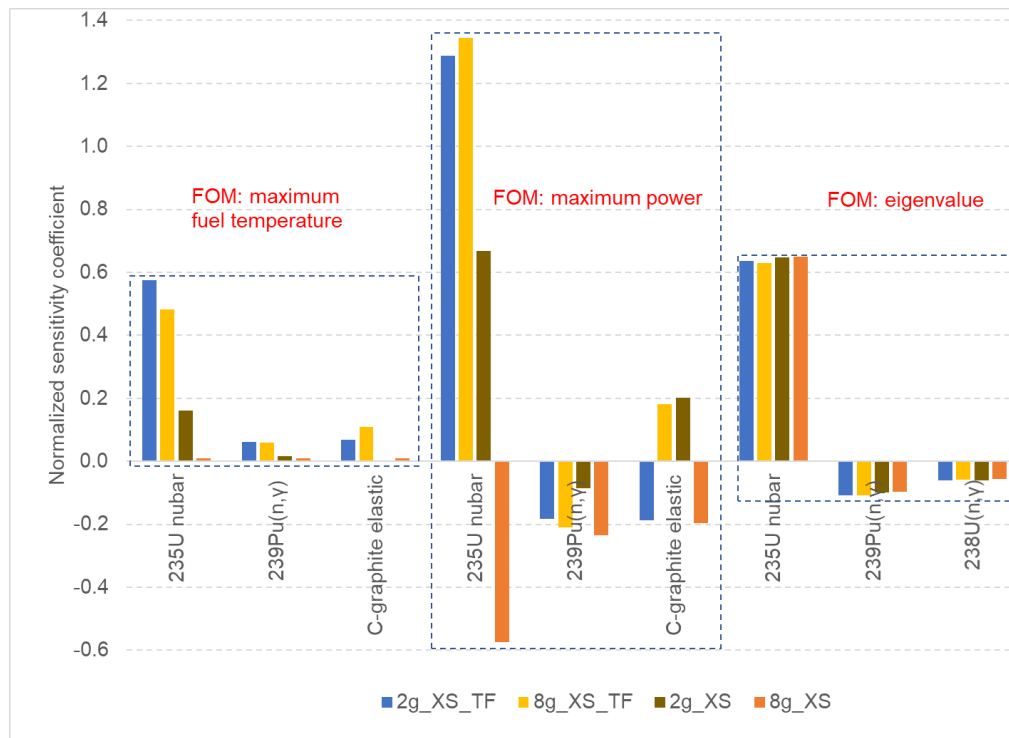


Figure 8-15. Comparison of 2- and 8-group NSCs for three FOMs and three perturbed cross-section reactions.

### 8.1.5 Exercise III-1 Conclusion

The uncertainty and sensitivity results obtained for three versions of the coupled steady-state exercise III-1 were presented in this section. The impacts of cross-section and thermal fluid and uncertainties were assessed in isolation by firstly coupling only the perturbed cross-section libraries with the nominal RELAP5-3D model (Exercise III-1a), followed by the perturbed RELAP5-3D models with the nominal PHISICS model (Exercise III-1b). The main objective was the combined uncertainty assessment of both neutronics and thermal fluids input uncertainties (Exercise III-1c). As a secondary objective, the impact of core-model energy-group boundaries on FOM uncertainties were investigated by comparing the results obtained for the 2 and 8-group structures introduced in Chapter 7.

It was found that although the power distribution and control-rod worths are affected more significantly by cross-section uncertainties, the convective heat transfer via forced helium gas flow minimize the impact of these variations on the fuel temperatures. In general, the axial offset produced the largest standard deviations (1.3–2.9%), followed by the maximum fuel temperature (0.1–1.5%) and the power peaking (0.7–1.2%). The differences between the various steady-state models are the largest for the MFT, where the impact of the TF uncertainties can clearly be observed. The MFT standard deviations of the XS-only models are much lower (<0.1%) than the models that include TF perturbations, where standard deviations of up to 1.54% is calculated.

The fuel temperature standard deviations for Exercise III-1a are consistently significantly smaller than the standard deviation for the Exercise III-1b and III-1c models, indicating that the perturbation of cross-sections had a smaller impact on the fuel temperature than the perturbation of TF input parameters. The cross-section uncertainties produced a 0.2–2.0% standard deviation in the local power, but the addition of TF uncertainties caused significantly higher standard deviations (2.0–3.6%); especially in the upper region of the core where the peak power occurs. These uncertainties in local power and fuel temperature are significant enough to take into account during the design-margin assessment process, but it is lower than the historic values assumed by GA of up to 15% in fuel temperatures and 10% in local power (Baxter, 2010)<sup>55</sup>. The value of the BEPU approach vs. very conservative assumptions is therefore illustrated by this comparison.

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<sup>55</sup> These 10-15% estimates included all sources of uncertainties, and since the tools and modeling approaches available to GA in the 1980s probably resulted in larger code/methodology uncertainties compared to the current study, it cannot be compared directly to the values determined in this work. The current study also utilizes significant model assumptions and simplifications (Appendix B-1) that would add at least a few percent to the power and temperature uncertainties.

In terms of the sensitivity assessment, the NCSs for uncertainties in the maximum power are particularly sensitive to the number of groups utilized, but the impact on the MFT is minimal because the convective heat transfer via forced helium flow disconnects the regions in the core where the maximum power is generated (FR3 second block from the top) and where the MFT occurs (FR1 bottom block). However, it was concluded that even if a 2-group model could be acceptable for use in scoping-level best-estimate and uncertainty assessments, the sensitivity of local parameters like the MFT and especially the maximum power peaking requires a higher number of energy groups that are optimized to capture the physics of the  $^{238}\text{U}(n,\gamma)$  and  $^{239}\text{Pu}(n,\gamma)$  resonance regions.

In general, the value and ranking of most PCCs and NSCs are very similar regardless of the perturbed-input data (TF, XS or both). For the coupled Exercise III-1 models, the covariance (uncertainty) in the  $^{235}\text{U}(\bar{\nu})/^{235}\text{U}(\bar{\nu})$  reaction again dominates the eigenvalue, MFT, and maximum power uncertainties, followed by the  $^{239}\text{Pu}(n,\gamma)/^{239}\text{Pu}(n,\gamma)$  reaction. Overall, the reactor boundary conditions still dominate the MFT and maximum power uncertainties.

## 8.2 MHTGR-350 Exercise IV-2: Coupled Transient Core Neutronics and Thermal Fluids

The propagation of input uncertainties in cross-sections, operational boundary conditions (model boundary conditions) and thermal fluid and material properties is concluded with the CRW coupled transient. The CRW is a reactivity-insertion transient typically included in HTGR safety-case analysis, and GA analysed a similar transient as part of their PSID (Stone & Webster Engineering Corporation, 1986).

### 8.2.1 Specification of the IAEA CRP on HTGR UAM Exercise IV-2 and Modeling Approach

In terms of the current work, the Exercise IV-2 transient is based on the three sub-exercises, III-1a, III-1b, and III-1c, discussed in Section 8.1.1, and is defined in the draft IAEA CRP specifications (Strydom 2018) as a coupled core transient at HFP conditions with combined feedbacks between power, temperatures, and neutron kinetics. Perturbations of kinetic parameters such as beta-effective and delayed-neutron yields are not included in the current work because covariance data on these parameters are not yet available in SCALE 6.2. The transient models used for this CRW transient are identical to the five steady-state models discussed in Section 8.1.1. The transients start at the end of the converged steady-states by utilizing the restart capability of P/R.

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A null transient (i.e. with no change in model input parameters) is performed at the start for a period of 100 seconds to ensure a stable condition is reached after normalization by the eigenvalue<sup>56</sup>. This is followed by the withdrawal of all control rods from the bottom of the fifth fuel block to the top of the first fuel block (395 cm) over a period of 200 seconds, as shown in Table 8-5.

The relatively slow CRW rate of 1.975 cm/s was chosen to ensure that this event stays below the prompt-critical threshold by inserting approximately 0.6%  $\Delta k/k$ . The transient was then followed for another 300 seconds, for a total time of 600 seconds, primarily to observe the turnaround point in fuel temperatures. Another reason for the selection of a relatively slow CRW rate is related to limitations of the current RELAP5-3D fuel-temperature model. As indicated in Appendix B-1, the RELAP5-3D fuel temperature is represented as the volume-homogenized heat-structure temperature of six fuel blocks in FR1 for each axial layer, and eight fuel blocks each in FR2 and FR3. As a typical system code model, this ring approach is not capable of resolving the temperature of either the UCO fuel kernels, the 220 fuel compacts, or even a single-block fuel temperature.

Because the fuel, compact- and block-graphite negative temperature-reactivity feedbacks are responsible for the turnaround in fission power, the underestimation of these temperatures caused by volume homogenization would lead to higher power peaks and slower responses than a more-accurate temperature model would predict (Strydom 2016, Ortensi 2009). By therefore limiting the reactivity insertion to the sub-prompt-critical domain, the change in power occurs relatively slowly, which allows the current approximated model predictions to be remain acceptable, especially if the focus is on the relative uncertainties between the various models and inputs.

Table 8-5. Description of Exercise IV-2 control-rod withdrawal event.

| Time (s) | Description                                                                                                     |
|----------|-----------------------------------------------------------------------------------------------------------------|
| 0–100    | Null transient phase; no change in model parameters.                                                            |
| 100-300  | Withdraw control rods at 1.975 cm/s from 395 cm (bottom of fifth fuel block) to 0 cm (top of first fuel block). |
| 300-600  | Track core power and fuel-temperature evolution.                                                                |
| 600      | End of transient.                                                                                               |

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<sup>56</sup> Transient solvers usually require normalization by the steady-state eigenvalue in a source-driven transport formulation to ensure that the transient starts with zero reactivity.

### 8.2.2 Exercise IV-2 Uncertainty Results

It was shown in the preceding chapters that the use of two energy groups leads to significant differences compared to the 8- and 26-group PHISICS models for best-estimate calculations, but also that the uncertainty and sensitivity data were sufficiently similar to justify the use of two groups for early scoping studies, for which faster calculation performance is important. In addition to the propagation of cross-section and TF input uncertainties, a comparison of the 2- and 8-group best-estimate and U/SA results are again performed to assess whether these earlier observations and conclusions remain valid for a strongly coupled reactivity transient.

The change in the mean MFTs during the CRW transient are shown in Figure 8-16. As noted in Section 8.1.4, the 8-group MFT starts off 20 K (1.6%) higher than the 2-group temperatures and remains higher throughout the transient. The MFT differences between models that used perturbed cross-sections and thermal fluids are less than 5 K (0.5%) for the 2-group models while the 8-group MFT data sets (8g\_XS and 8g\_XS\_TF) are identical.

Because the MFT is a spatially dependent parameter (that is, it changes location over time depending on the core state), the spatial variances in the mean MFT and power and their standard deviations are again of interest. The full fuel temperature and power spatial data set is provided in Table D-6, but an example of these data is shown for the FR1 mean fuel temperature in Figure 8-17 at the time point when the peak fuel temperature is reached ( $t = 370$  seconds in Figure 8-16). The 20–30 K difference between the 2- and 8-group results can be seen here as well, with a slightly increasing trend towards the hotter bottom region of the core. The axial fuel temperature profile of the 8-group XS\_TF model at  $t = 100$  seconds—i.e. before the start of the CRW—is also included in this figure to allow a comparison of the spatial effects of the CRW event.

The large increase (125 K or 15%) in the colder top region of the core can clearly be observed, compared with the much-smaller increase in the bottom fuel temperatures (40 K or 3.3%). This is caused by the withdrawal of the rods in the upper core region and the resultant local power increase here. The impact of energy-group structure on the mean MFT is thus significantly larger than the impact of uncertainties in the cross-sections or TF properties.

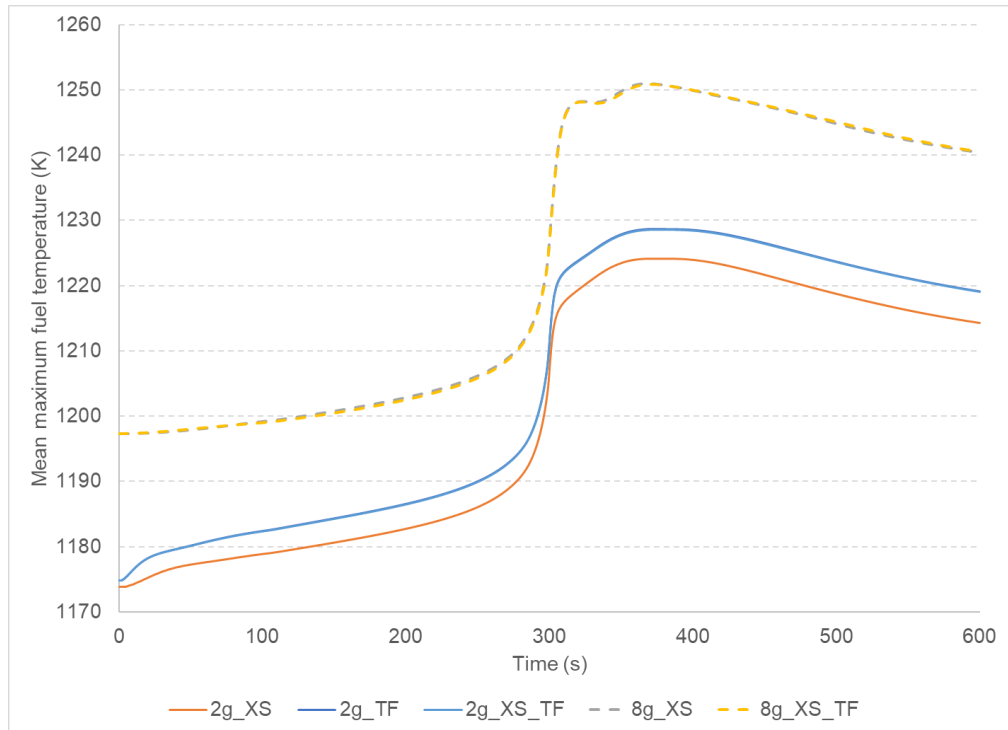


Figure 8-16. Comparison of mean MFT (K) for perturbations of XS only, TF only, and both XS and TF.

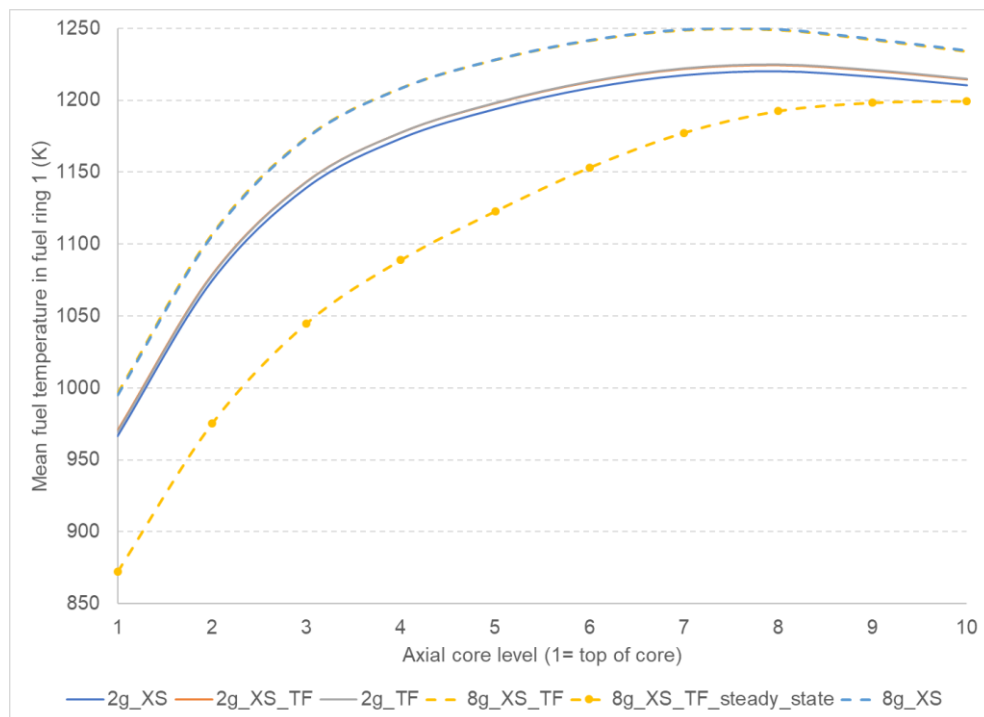


Figure 8-17. Comparison of mean fuel temperature (K) axial profiles in FR1 at 0 and 370 seconds.

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In terms of changes in MFT standard deviations, the same trends can be identified in Figure 8-18 as were discussed for the steady-state results in Section 8.1.3. The models that included the propagated TF and boundary-condition uncertainties again produced the largest uncertainties (up to 1.67%), with the differences between the 2- and 8-group models likewise insignificant. The data are shown here for the period 200–400 seconds because the MFT uncertainties remain relatively constant for the duration of the CRW event.

Uncertainties in the cross-sections had a much-smaller impact on MFT uncertainty ( $<0.25\%$ ), and the slight overestimation of the 2-group model observed for the steady-state is maintained for the duration of the CRW. It is interesting to note that the large increase in fission power did not lead to a change in the difference between the 2- and 8-group models; i.e. the trends identified in Section 8.1.3 remain applicable to this strongly coupled transient as well.

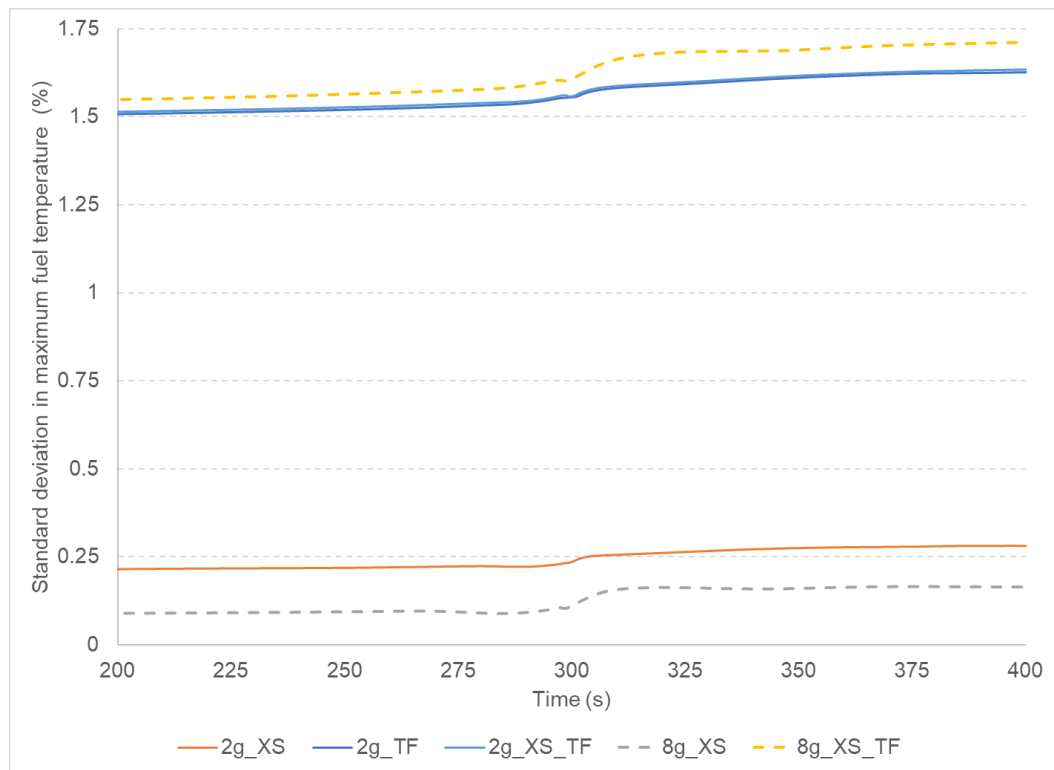


Figure 8-18. Comparison of MFT standard deviation (%) for perturbations of the cross-sections only, thermal fluids only, and both cross-sections and thermal fluids.

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The spatial standard-deviation data sets are also included in Table D-6 and Table D-7 for reference purposes. The axial profiles of the fuel-temperature standard deviation for FR3 at  $t = 370$  seconds are compared in Figure 8-19, where it can be seen that models with cross-section perturbations only predicted a decrease from the top to the bottom of the core while the models that included the uncertainties from both TF and cross-sections showed a slightly smaller inverse trend.

This increase in fuel-temperature uncertainty towards the top of the core is related to the large shift in axial-power production that occurs in the top regions of the core as the rods are removed from the core (as shown in Figure 8-20), where uncertainties in the cross-sections (specifically  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$ ) would play a larger role than in the bottom of the core.

The two metrics investigated produced opposite trends. For mean fuel temperatures, the model uncertainties related to the selection of different energy-group structures are larger (up to 3.05% in Table D-7) than the uncertainties caused by cross-sections or TF input parameters ( $<0.12\%$ )<sup>57</sup>. For the standard deviations of the mean fuel temperatures, the choice of energy-group structure is, for most of the locations, less important ( $<0.7\%$ ) than the inclusion of uncertainties in the TF input parameters (up to 1.50%).

The withdrawal of the control-rod bank resulted in a sharp increase in the mean reactor power caused by the insertion of positive reactivity, as shown in Figure 8-21. The maximum power is reached directly after the withdrawal of the rods are terminated at 300 seconds, with a small ( $<0.5$  s) delay between the 2- and 8-group model peaks (Figure 8-22). The 2-group models both produced 3.2% higher predictions of the mean maximum core power (825–850 MW) than the respective 8-group models (800–825 MW), most likely caused by differences in the local temperature-to-power feedback cycles. It is also noteworthy that the difference in the mean maximum power between the cross-section and combined cross-section/thermal fluid models are also approximately 25 MW (3.2%); i.e. the impacts of energy-group choice and uncertainties in the cross-sections and thermal fluids seem to be comparable in size.

However, this statement is only true for the *total* reactor power; an analysis of the spatial differences included in Table D-7 show that the addition of thermal fluid input uncertainties added consistent increases of 1.80–2.30% in the mean *local* power generated in each of the fuel-ring locations, compared to much-larger local power increases of up to 14.61% when the 2-group model is used instead of the 8-group model.

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<sup>57</sup> The MFT is not directly influenced by the choice of group structure, but because the primary influence of group structure is on the local power production, as discussed in Section 8.1.3, changes in the local power density will lead to linked changes in the MFT as well. This link can however be delayed or diluted as long as the forced helium flow decouples the regions where peak power and temperatures are produced.

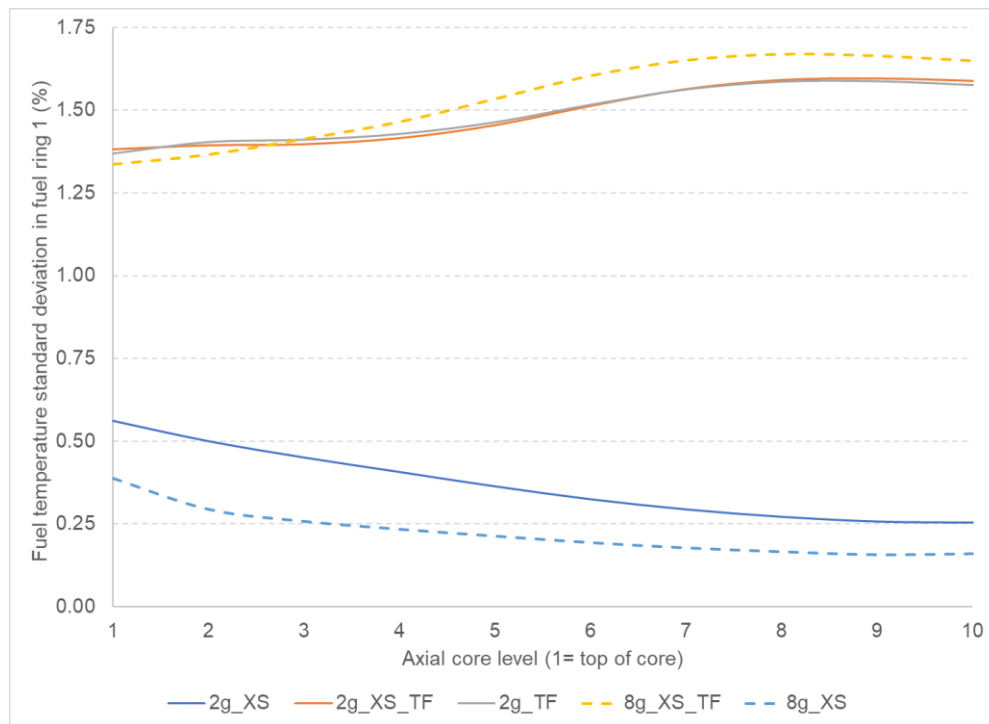


Figure 8-19. Comparison of mean fuel-temperature standard deviation (%) axial profiles in FR3 at 370 seconds.

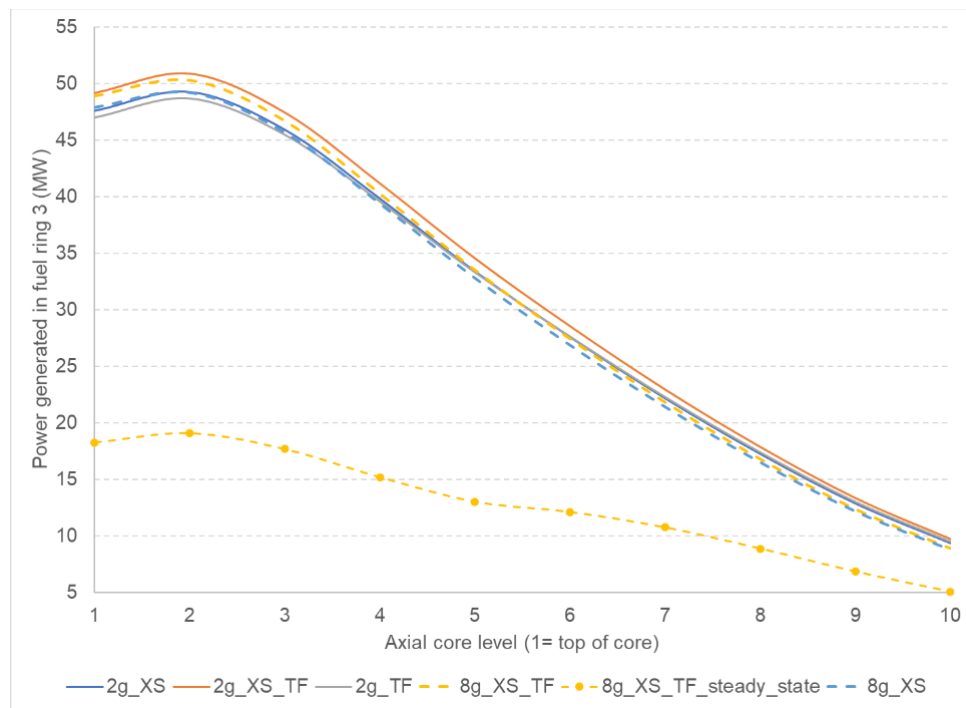


Figure 8-20. Comparison of mean power generation in FR3 (MW) at 300.5 seconds.

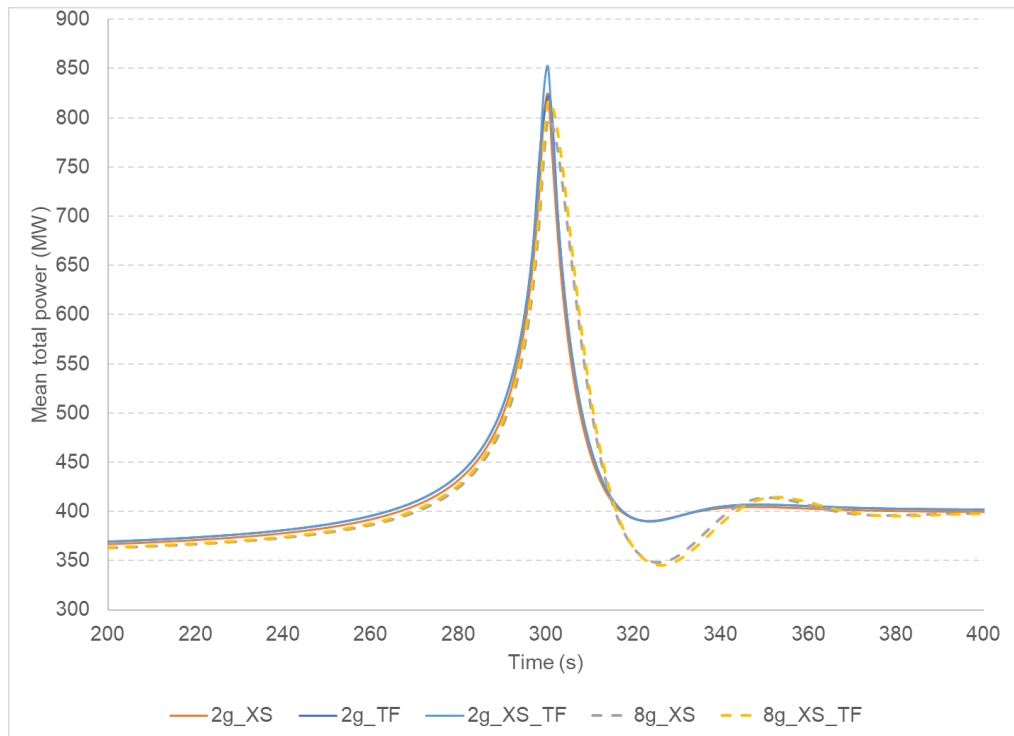


Figure 8-21. Comparison of mean total reactor power (MW) for perturbations of the cross-sections only, thermal fluids only, and both cross-sections and thermal fluids.

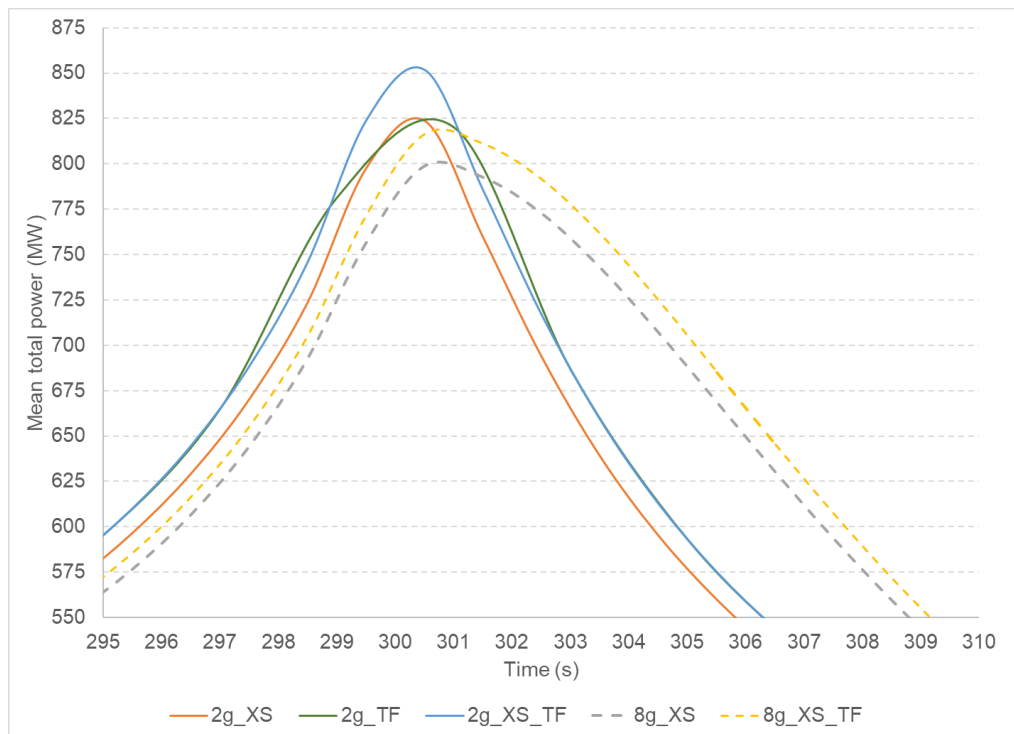


Figure 8-22. Detail of the mean total reactor power (MW) between 295 and 310 seconds.

The change in the total power standard deviation ( $\sigma$ ) is presented in Figure 8-23, where the large increase, especially in the cross-section only perturbed models after  $t = 280$  seconds, can clearly be seen. (The subsequent sensitivity analysis will identify the parameters most likely responsible for this significant increase). For most of the CRW transient the 2- and 8-group\_XS standard deviations remain much smaller ( $<0.50\%$ ) than the respective 2- and 8-group\_XS\_TF standard deviations, which essentially just continue the steady-state trends discussed in Section 8.1.3. The final 20 seconds of the CRW leads to an increase from  $0.50\%$  to almost  $3.0\%$  in  $\sigma$ , but the models that included the thermal fluid input uncertainties only increased by approximately  $0.5\text{--}1.0\%$ . All models predict a return to the pre-CRW values within 100 seconds following the termination of the CRW event.

The differences between the 2- and 8-group standard deviations remain significant enough to recommend the use of eight energy groups or more when possible, but even for such a large reactivity-insertion transient, it seems that the 2-group model can nevertheless provide first-order trends to the HTGR core designer who needs to perform early scoping calculations, especially if larger uncertainty margins can be tolerated<sup>58</sup>.

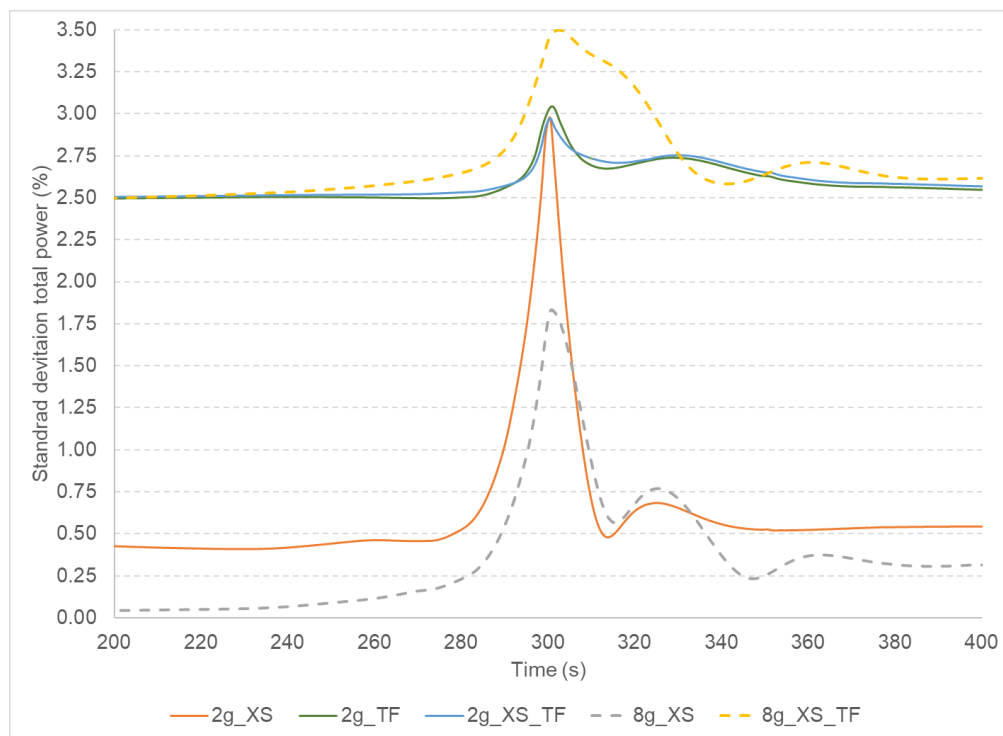


Figure 8-23. Comparison of total reactor power standard deviation (%) for perturbations of the cross-sections only, thermal fluids only, and both cross-sections and thermal fluids.

<sup>58</sup> A 3% (25 MW) uncertainty margin seems quite acceptable even for the later stages of core design.

The axial profiles of the FR3 local-power production are compared in Figure 8-24 at the time of maximum total reactor power (i.e., 300.5 seconds). Most of the models follow an increasing trend in the standard deviation towards the bottom of the core, i.e. as the mean local power decreases, uncertainty tends to increase. The 2g\_XS model produced a relatively flat axial profile, but in general, there is clearly more axial variation in the local-power standard deviations than the local-fuel-temperature standard deviations (Figure 8-19).

This is most probably related to large differences in the mean local powers and fuel temperatures between the top and bottom of the core: the rise in FR1 fuel temperatures amounts to 250 K (26%), compared to 42 MW (466%) for the local power in FR3 (Figure 8-20). It is also noted that peak power generation occurs 5 blocks (395 cm) higher than the MFT, and that the additional heat generated by the removal of rods in the upper parts of the core is continuously redistributed through convection and conduction to the lower regions of the core, effectively diluting the link between the fission-power increase that is generated in the upper core and the highest fuel temperatures near the bottom of the core.<sup>59</sup>

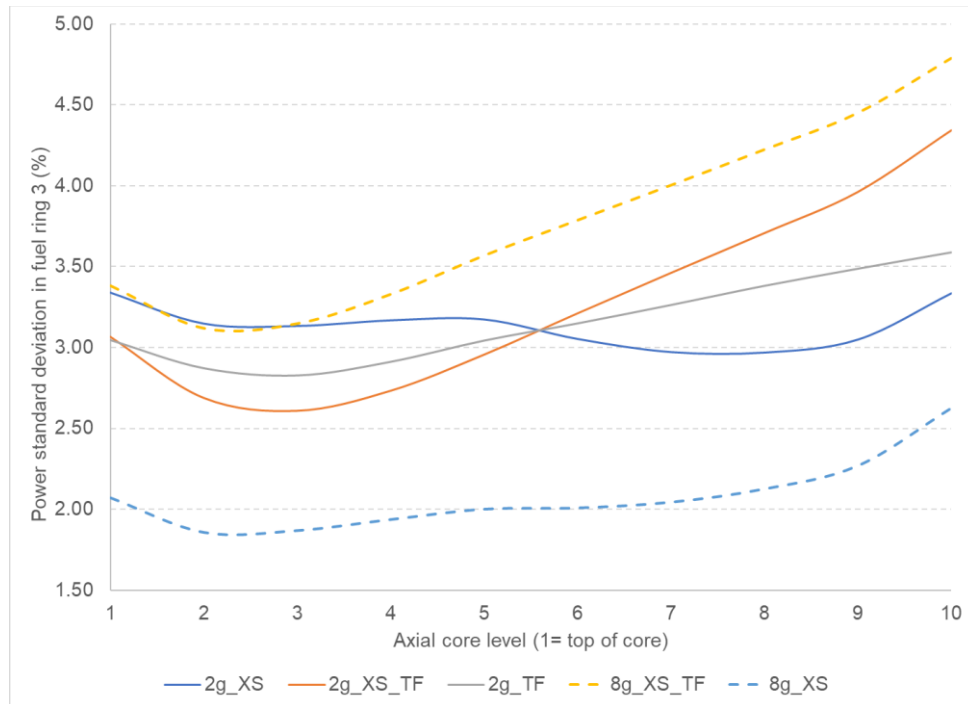


Figure 8-24. Comparison of axial-power standard deviation (%) profiles in FR3 at 300.5 seconds.

<sup>59</sup> The discussion in this section shows the risk in comparing only integral parameters (e.g. eigenvalue or total reactor power). Large spatial variances in the chosen metrics can be hidden by these integral values, and the CRW transient produced a good example of spatial decoupling between the locations where the peak power and peak fuel temperatures are generated.

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In summary, if trends in the spatial data shown in Table D-7 are compared, it can be concluded that:

- Mean values:
  - The choice of energy groups has a significantly larger impact on the local power (14.61%) than the local fuel temperatures (3.05%). The 2-group model mostly overestimated local-power generation but underestimated local fuel temperatures in large areas of the core.
  - The inclusion of thermal fluid uncertainties did not affect local fuel temperatures significantly ( $<0.12\%$ ), but local power generated was increased up to 2.27%.
  - The choice of energy-group structure therefore dominates the differences observed in both the mean local power and mean local fuel temperature. The same conclusion is reached as in earlier chapters: the 2-group best-estimate (and mean) local powers and fuel temperatures are significantly lower than the 8-group estimates, and should only be used for early scoping studies where these larger uncertainties can be tolerated.
- Standard deviations:
  - The inclusion of thermal fluid uncertainties has a significant impact on local-power standard deviations of up to 2.85% higher than only including cross-section input uncertainties. The local fuel-temperature standard deviations are also impacted to a lesser degree ( $<1.51\%$ ).
  - The choice of the 2-group model leads to much-lower underestimations of standard deviations of the local power ( $<0.70\%$ ). The energy-group structure did not affect the local fuel-temperature standard deviations ( $<0.1\%$ ).
  - For estimates of the standard deviations (uncertainties) in the local power and fuel temperatures, a 2-group structure can still be utilized to produce realistic transient trends, but the inclusion of thermal fluid input uncertainties is essential, especially for local PP estimates. This conclusion is again similar to the earlier conclusions reached for Exercise II-2 in Section 6.2.2 and Exercise III-1 in Section 8.1.4, and remains an important contribution of this work to HTGR U/SA. It could be of interest to HTGR core designers if the expense of more than two groups are taken into account when many transient studies with perturbations need to be performed.

### 8.2.3 Exercise IV-2 Sensitivity Results

For the thermal fluids stand-alone PLOFC transient, it was found in Section 7.5.2 that the uncertainties in reactor operating conditions (that appear as model boundary inputs on the P/R model) are responsible for most of the observed uncertainties in the MFT. During the later stages of transient uncertainties, decay heat and the thermal conductivity of H-451 reflector graphite became more important than these boundary-condition uncertainties, but in general, the inclusion of bypass-flow and material-property uncertainties were not as important. The objective of this section is to compare the ranking and impact of these uncertainties for the coupled CRW transient, in addition to assessing the propagated effects of cross-section uncertainties in combination with the thermal fluid and boundary-condition uncertainties.

Continuing the approach followed for the coupled steady-state Exercise III-1, RAVEN is again used to calculate NSC and PCC metrics for an integral FOM (total reactor power) and a local spatial FOM (MFT). The sensitivity parameters are likewise compared for the 2- and 8-group models with XS-only perturbed-input data, TF-only perturbed-input data, and both XS and TF perturbed-input data to determine whether earlier observations and conclusions are still valid for the strongly coupled CRW transient.

The sensitivity analysis of a coupled transient is complicated by the volume of time-dependent nature of the integral and spatial data available because spatially dependent “snapshots” of the MFT and power density can be taken at any time during the event. In the discussion that follows, the time at which peak power (300.5 s) and MFT (370.0 s) are reached will be used to compare PCC and NSC data. In the interest of a concise analysis, the focus is mainly on the sensitivity-coefficient data, and only the main results will be included in this section. Supplementary data are provided in Appendix D.

The change in the PCC data for total core power in the period 200–400 seconds into a CRW event are shown in Figure 8-25. As observed for the Exercise III-1 steady-state, measurement uncertainties in the total reactor power ( $\sigma = \pm 1\%$ , see Table 7-2) produced the most-significant linear correlation for the total power produced during the CRW. Uncertainties in the mass-flow rate and inlet-gas temperature ranked second and third, respectively.

Regarding the impact of uncertainties on total reactor power, there is a noticeable increase in the degree of linear correlation between these two input uncertainties and power (Figure 8-25) during the last 20 seconds of the CRW event when the total power increases very rapidly and the importance of additional heat removal increases. The same trend can be seen in Figure 8-26 for the NSC data set.

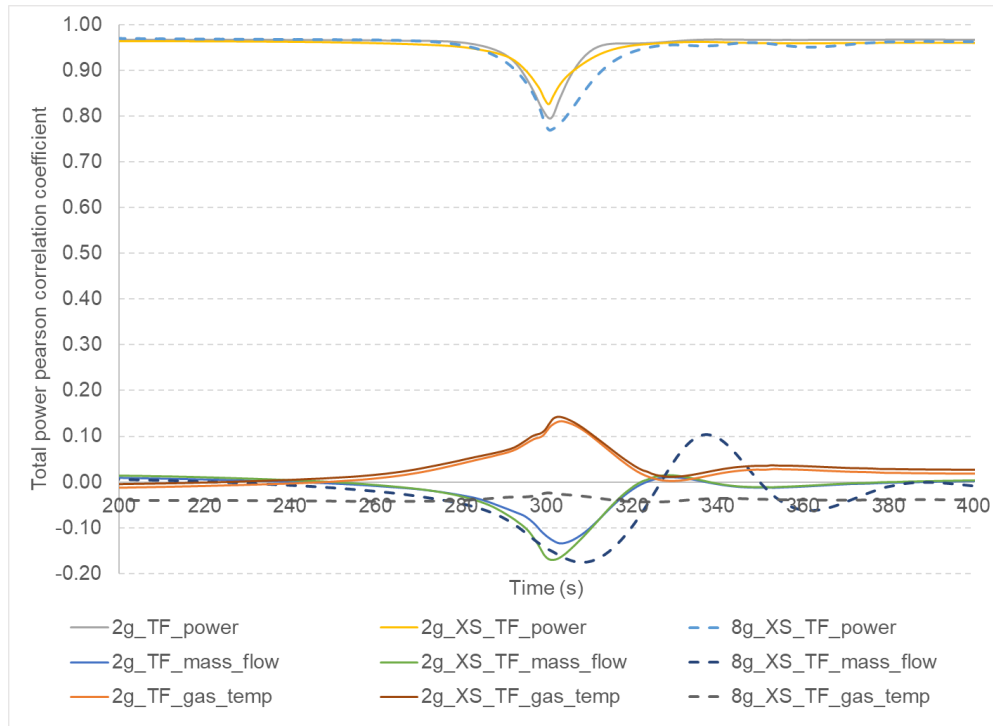


Figure 8-25. Comparison of 2- and 8-group total power PCCs for the CRW transient between 200 and 400 seconds. Data shown for three perturbed model variants.

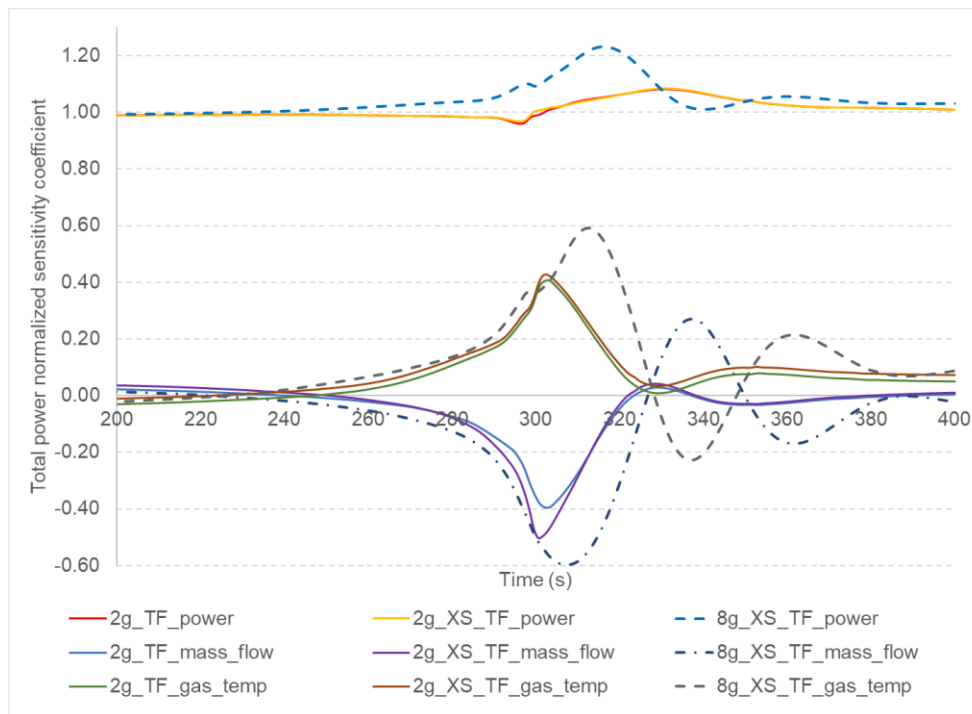


Figure 8-26. Comparison of 2- and 8-group total power NSCs for the CRW transient between 200 and 400 seconds: reactor operational boundary-condition uncertainties.

## CHAPTER 8: MHTGR EXERCISE III 1 AND IV 2: COUPLED CORE NEUTRONICS AND THERMAL FLUIDS STEADY-STATE AND CRW TRANSIENT

The only (minor) difference between the 2- and 8-group data sets is the prediction of a damped oscillation in mass-flow rate PCC of the total power FOM for the 8g\_XS\_TF model, which is not observed for the 2-group model. This is primarily caused by the inclusion of more epithermal energy groups that allow improved modeling of the  $^{238}\text{U}$  and  $^{239}\text{Pu}$  resonance-absorption regions, as well as thermal upscatter within the four thermal-energy groups.

The NSCs shown Figure 8-26 can be expressed in multiple ways. RAVEN calculates NSC as sensitivities normalized to the mean values (see Appendix B-1); i.e. the default RAVEN NSCs are “mean”-normalized sensitivity coefficients. These NSCs are useful in the sense that they represent a per-unit sensitivity metric; e.g. in the linear formulation, an NSC of 0.5 implies that a perturbation of +1% in the inlet-gas temperature will lead to a change of  $0.5 \times 1\% = 0.5\%$  in the mean MFT. By multiplying the NSC coefficients with the MFTs or total power calculated during the transient, the sensitivity coefficients can therefore also be expressed in physical units—e.g. the change in fuel temperature (K) for a change of 1%<sup>60</sup> in the input parameter of interest<sup>61</sup>.

It is important to note that this metric is *not* the contribution of a specific input parameter to the overall uncertainty in the FOM<sup>62</sup>, but an indication of how much the FOM would change if only that parameter were varied with 1%. The goal of calculating and ranking these sensitivity coefficients is to provide the HTGR core designer with an indication of where the focus could be if a reduction in simulation-model uncertainties is desired.

An example of such a conversion between the two NSC types is shown in Figure 8-26 and Figure 8-27, where the total power sensitivity coefficients for the three boundary-condition input uncertainties are compared. The conclusions and trends that can be drawn on both of these sensitivity-coefficient types are obviously identical, but the expression of sensitivity coefficients in terms a physical parameter (MW) might be of more-practical value to an HTGR core designer.

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<sup>60</sup> The “unit” can also be expressed as the change in the FOM per *standard deviation* of the input parameter, i.e.  $\Delta T/\Delta\sigma$  instead of  $\Delta T/\Delta\%$ .

<sup>61</sup> Since RAVEN has access to the P/R perturbation factors for all inputs and to the outputs for all 1,000 CRW transients, it can assess how much the fuel temperature would change for a unit change in any of these input parameters. This is equivalent to the standard one-by-one brute-force sensitivity analysis approach.

<sup>62</sup> As noted in Section 0, a variance-based sensitivity method, such as Sobol’s, would need to be used to determine the actual contributing components to the overall uncertainty. This aspect is beyond the scope of the current work, but it is listed as possible future contributions to the HTGR U/SA field in Section 9.2.

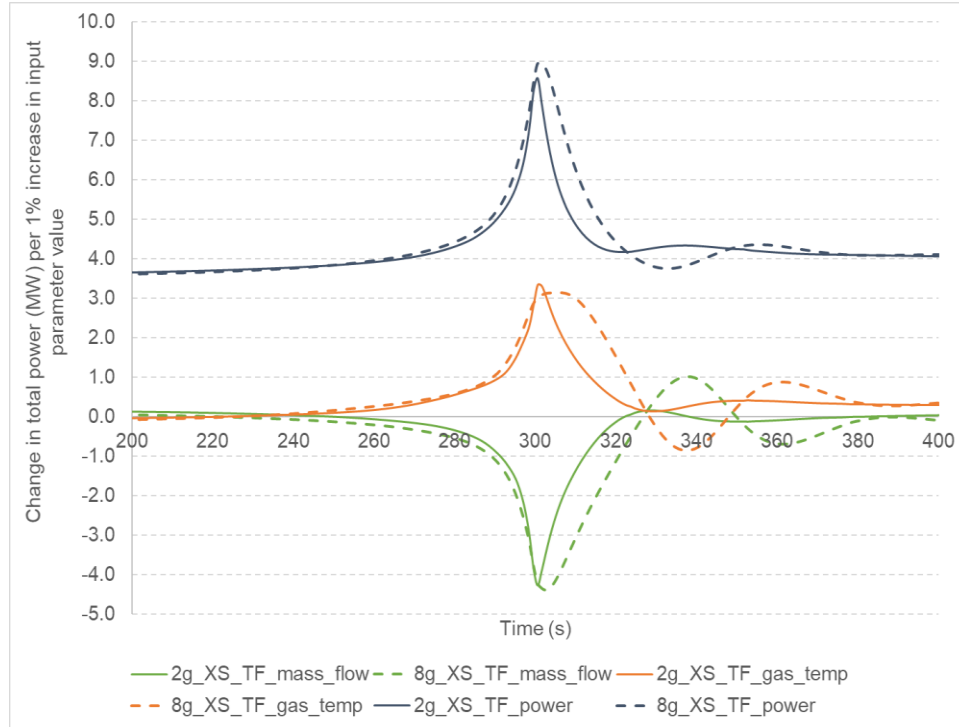


Figure 8-27. Comparison of 2- and 8-group total power sensitivity coefficients (MW/%) for the CRW transient between 200 and 400 seconds: reactor operational boundary-condition uncertainties.

It can be seen in Figure 8-27 that, at  $t = 300$  s, an increase of 1% in the reactor-power *input* variable in the P/R model (to 353.5 MW) would result in a change of 9 MW in the predicted core power *output* during the CRW transient. An increase of 1% in the inlet mass-flow rate (to 158.7 kg/s) would, however, produce less than half this increase ( $\sim 4$  MW) in the core power output. In this simplified example, it is more beneficial, therefore, to spend resources on decreasing the measurement uncertainty in the total reactor power than the inlet mass-flow rate. (In operating reactors, the two variables are usually related through a calibration scheme that equates the flux and fluidic power measurements to the desired secondary side power output.)

Apart from the damped oscillations already observed for the PCCs as well, the 2-and 8-group sensitivity coefficients do not differ significantly (in MW units) although some larger differences are observed for the normalized NSCs at  $t = 315$  seconds.

Because the use of two energy groups leads to a loss of fidelity on these statistical-sensitivity indicators, more than two groups are recommended for accurate U/SA analysis. If the costs of higher energy-group calculation are prohibitive during early design simulations<sup>63</sup>, a 2-group model could still be useful if less-accurate trend predictions can be tolerated.

The total power sensitivity coefficients calculated for the four cross-section reaction pairs previously investigated in Section 8.1.5 are presented in Figure 8-28. In terms of the impact on the total power as FOM, the largest sensitivity coefficient is obtained for the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  reaction pair: an increase of 1% in the Sampler  $Q_{x,g}$  multiplication factor for the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  reaction would produce 10 MW more power at the peak of the CRW, compared to the  $Q_{x,g}$  factor for the second ranked cross-section C-graphite (n,n') / C-graphite (n,n') elastic-scatter reaction that would produce 2.5 MW.

The uncertainty in the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  reaction also seem to be ranked above the total reactor power input uncertainty in terms of impact on the reactor power output, but only on a normalised “1%” change basis. In reality, the covariance of the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  is smaller than this, and is expressed in Sampler as shown in Figure 3-7. A perturbation of 1% in this reaction is equivalent to 2.5 times the Sampler population standard deviation, whereas the same 1% perturbation in the total reactor power measurement is worth  $1\sigma$ . Regardless of the ranking order, it is nevertheless clear that the uncertainty in the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  reaction play a very important role in the output uncertainties of several important FOMs in HTGR analysis.

This trend is similar to the Exercise III-1 steady-state data shown in Figure 8-13: the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  uncertainty is ranked first for a similar integral parameter (eigenvalue), and second for the local maximum power density. The  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  uncertainty is also identified by Hou et al. (2019) as the most-important contributor for the LWR UAM Phase I results.

However, it is also noticeable in Figure 8-28 that the inclusion of TF uncertainties in the sampled data set increases the total power sensitivities of the nuclear data (the dotted vs. solid lines in the plot). This might be related to three features of the statistical method followed in this work:

- The degree of linear correlation between the input and output parameters is given by the PCCs, which are relatively small ( $<0.05$ ) for most of the cross-section reactions. This implies that the uncertainties in sensitivity coefficients (calculated based on this linear assumption) are relatively high, i.e. the sensitivities become less accurate.

<sup>63</sup> A single 8-group CRW simulation with the coupled P/R model requires ~2 hours on a 32-processor node for 600 seconds simulation time. If e.g. 200 perturbations must be performed for five core models, the calculation cost for 1,000 CRW simulations are non-trivial, unless large cluster resources are available. The P/R calculation costs scale linearly with energy groups, i.e. an 8-group calculation will take approximately four times longer than a 2-group calculation. The use of a 2-group model, therefore, becomes attractive during the scoping core-design phase.

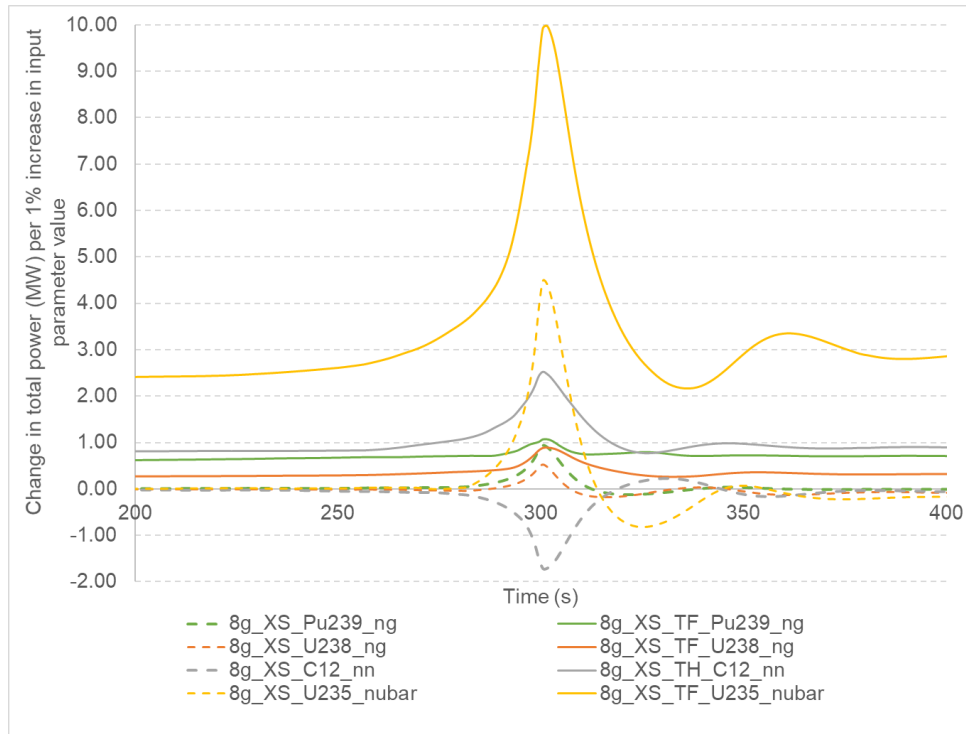


Figure 8-28. Comparison of 8-group total power sensitivity coefficients (MW/%) for the CRW transient between 200 and 400 seconds: cross-section uncertainties.

- The sensitivities are also dependent on the size of the statistical sample. It could be the case that the current sample size of 1,000 is not sufficient to resolve these sensitivities with a high degree of confidence.
- The linear-regression model used by RAVEN to calculate sensitivity coefficients assumes independence between the cross-section input uncertainties and the TF boundary conditions. For most of the parameters in this work, this assumption is acceptable—e.g. uncertainties in the mass-flow rate is independent of the  $^{238}\text{U}$  capture cross-section—but in the case of the total reactor power and  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ , there is a correlation in the sense that the  $^{235}\text{U}$  neutron yield per fission is one of the major contributors to the total neutron-reaction rate at any given time, which eventually equates to total reactor power. The uncertainty and covariance in this reaction will, therefore, be an important contributor to core reactivity. (Similar correlations might exist between the removal terms [the capture reactions] and total power as well, but it is probably weaker correlations that the neutron yield.)

In the PHISICS solver scheme, the total reaction rate is normalized to the user-input power for the steady-state transport solution, so that a P/R calculation that sampled both the  $^{235}\text{U}(\bar{v})$  yield and the total reactor power (as a model input parameter) could create a secondary dependency between these two parameters that might lead to inaccurate estimates of the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  sensitivity coefficients. The differences observed in Figure 8-28 for models that include both cross-section and thermal fluid uncertainties (XS\_TF) might therefore be distorted by these non-linear dependencies.

Because the focus of the present work is primarily on the uncertainty quantification application example, rather than a full sensitivity assessment (because a variance-based global sensitivity method is not deployed), the current sensitivity results obtained should be taken as indicative of trends, rather than high-confidence, high-accuracy sensitivity indicators.

The development of a rigorous sensitivity assessment statistical methodology applied to HTGRs could be an area of possible future research. An example of such a recent scheme developed for SFR designs can be found in the work of Bostelmann (2020). Up to now, current attempts at developing sensitivity assessment capabilities have been exclusively focused on neutronics stand-alone cases. The assessment of coupled TF sensitivity analysis is still an outstanding challenge in the author's view.

The designation *8g\_XS\_U238\_ng* in Figure 8-28 identifies data shown as belonging to the  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  reaction for the 8-group model that only utilized perturbed cross-sections. In total, there are 56 energy- and time-dependent PCC and NSC data sets available for each of the four nuclide-reaction pairs discussed in this work. The summary data in Table D-8<sup>64</sup> represents the maximum and minimum values calculated for all 56 covariance groups and over the duration of the CRW transient. (Note that Table D-8 reports NSC data to allow direct comparison with the NSC values in the earlier chapters of this work). It is shown in this table that the reactor power NSCs of the three cross-section reaction pairs are lower than the impact of the three boundary-condition uncertainties. The same observations can also be made by comparing the sensitivity coefficients in Figure 8-27 and Figure 8-28.

Due to limited space, the total power PCC and NSC data for uncertainties in the material properties (fuel and graphite specific heat, thermal conductivity) are not included in this table; all of these values were lower than the cross-section PCC and NSC values.

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<sup>64</sup> The detail data in the tables are included in Appendix D to allow a more streamlined discussion here.

Based on the results obtained in this section (and within the limitations indicated), it would therefore seem that a focus on improving measurement uncertainties in the prompt and delayed neutron-release per fission ( $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ ) reaction, as well as reactor power, inlet mass-flow rate and helium temperature measurement would yield the best results.

In contrast to the trends observed for total power, the degree of linear correlation (PCC) of uncertainties in the three boundary parameters on the MFT do not change during the CRW (Figure 8-29). As mentioned in Section 8.2.2, this is caused by spatial decoupling of the large rise in power in the cold upper region of the core and the diffused increase towards the hotter, bottom node where the MFT occurs. An 1% change in total power is worth approximately a 7 K increase in the MFT (Figure 8-30), closely followed by the sensitivities in the mass-flow rate (-6.5 K/%) and inlet-gas temperature (6 K/%). Similar to the impact on the total power, the highest-ranked input uncertainty on the MFT is again the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction, peaking at 7.5 K/% (as shown on the secondary y-axis of Figure 8-31). The impacts of uncertainties in the C-graphite (n,n') / C-graphite (n,n'),  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  and  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  cross-sections are ranked fourth through sixth, respectively. A ranking based on the minima and maxima of the MFT PCC and NSC data sets can also be found in Table D-8.

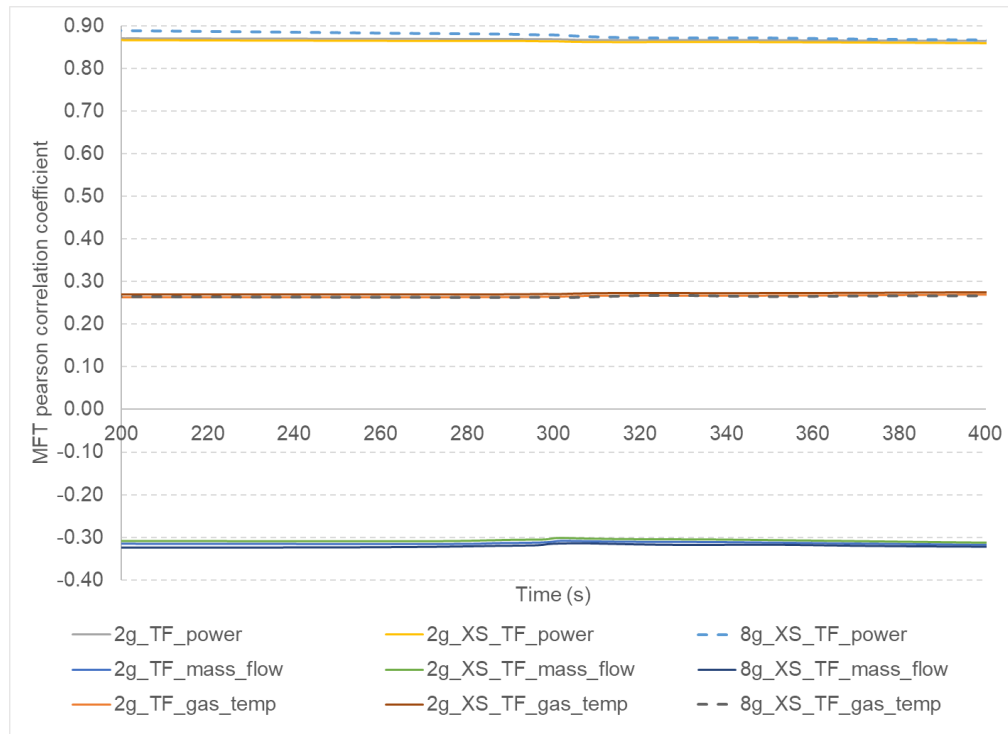


Figure 8-29. Comparison of 2- and 8-group MFT PCCs for the CRW transient between 200 and 400 seconds.

## CHAPTER 8: MHTGR EXERCISE III 1 AND IV 2: COUPLED CORE NEUTRONICS AND THERMAL FLUIDS STEADY-STATE AND CRW TRANSIENT

Similar to the trend noted for total power, it can again be seen that the addition of TF uncertainties in the sampled data set did not have a significant effect on the PCCs and sensitivity coefficients for the boundary conditions (Figure 8-29 and Figure 8-30), but significant differences can be seen for the cross-section data shown in Figure 8-31. Although the link between the MFT and the perturbations in the cross-section uncertainties seem less direct (i.e. the independence assumption might seem more valid), the addition of heat transfer through conduction and convection results in additional non-linear correlations that could lead to less-accurate MFT sensitivity coefficients.

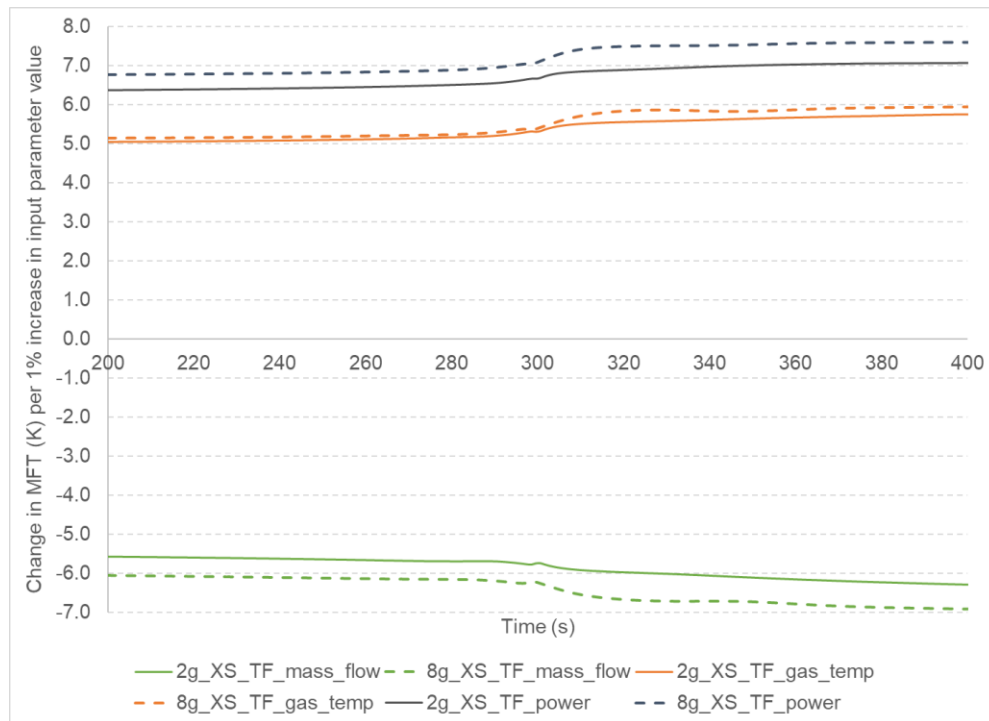


Figure 8-30. Comparison of 2- and 8-group MFT sensitivity coefficients (K/%) for the CRW transient between 200 and 400 seconds: operational boundary conditions uncertainties.

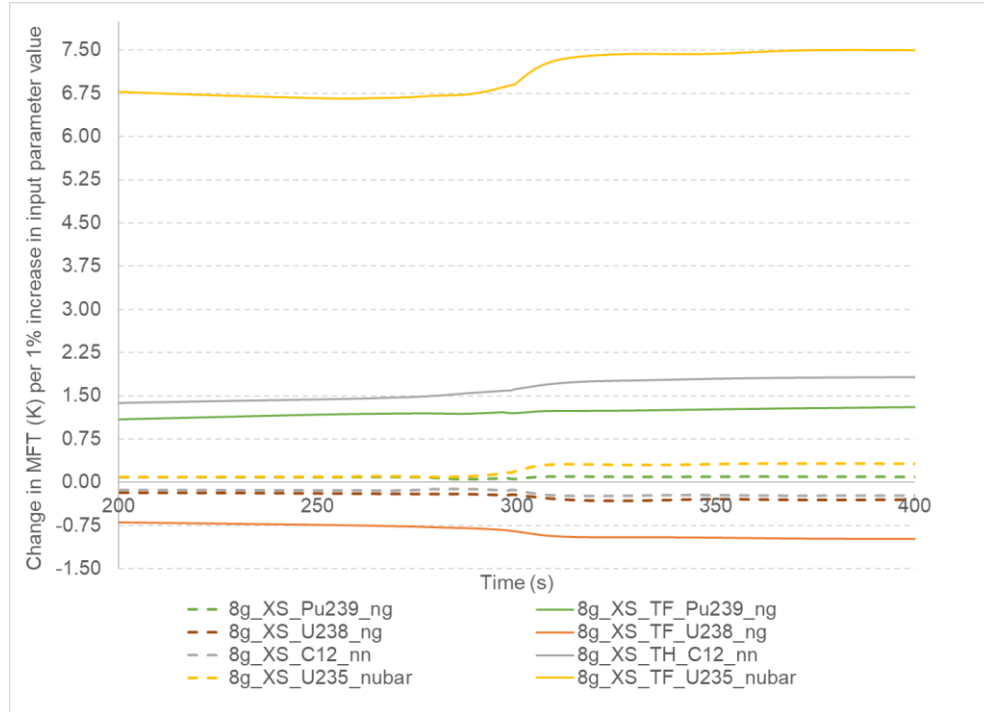


Figure 8-31. Comparison of 2- and 8-group MFT sensitivity coefficients (K/%) for the CRW transient between 200 and 400 seconds: cross-section uncertainties.

The main advantage of NSCs is that they allow direct comparisons in terms of relative (%) impacts on the FOM mean values. The power and MFT NSC results for the top-two input-parameter sensitivities ( $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ ) and reactor power) are shown in Figure 8-32. The main observations listed below are similar to trends identified for the coupled steady-state Exercise III-1 models:

- The uncertainties in total reactor power influences the *mean* of total power during the CRW much more than the influence on the mean MFT (NSC values of 1.2% vs. 0.6%).
- The power NSC oscillations follow a rise and fall in power, but the MFT NSC does not due to the decoupling between peak power and peak fuel-temperature locations and the effects of heat transfer via conduction and convection.
- The uncertainty in  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  leads to much-larger NSCs for power than for MFT when only perturbed cross-section models are used (dotted lines). This difference remains when TF uncertainties are included, i.e. the difference between solid lines and difference between dotted lines are the same.

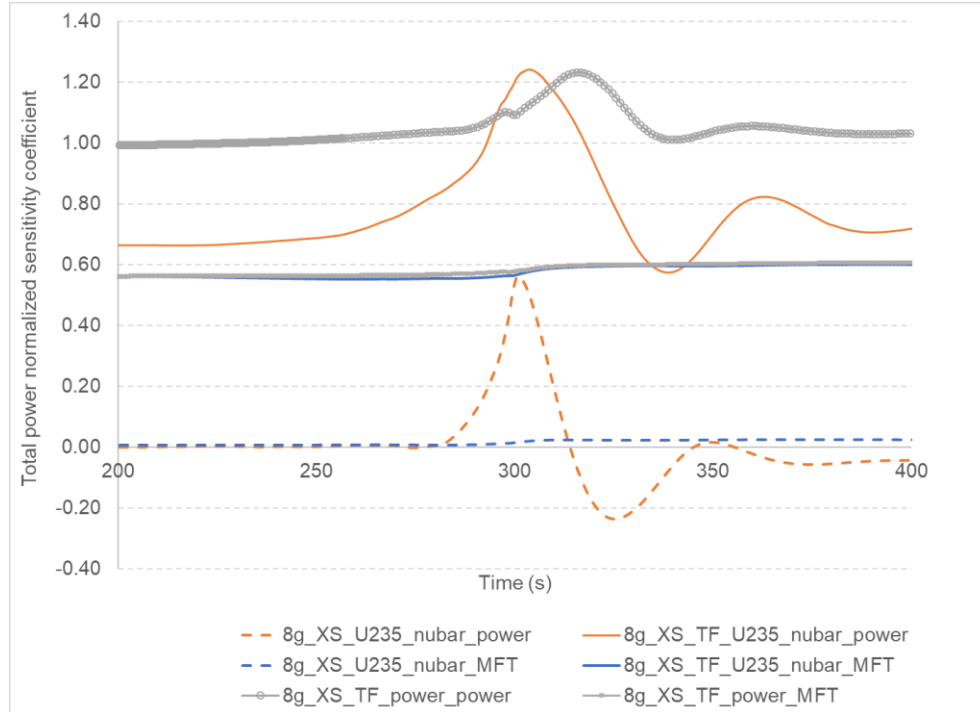


Figure 8-32. Comparison of 8-group power and MFT NSCs for the CRW transient between 200 and 400 seconds.

#### 8.2.4 Exercise IV-2 Conclusion

The CRW transient was used in this work as an example of a coupled neutronics and thermal fluid simulation that is required as part of a typical HTGR safety case. In the context of the applied statistical U/SA methodology, the CRW represents the conclusion of the SCALE/Sampler-propagated cross-section uncertainties from the lattice to the full-core phases. In order to isolate impacts of cross-section and TF input uncertainties separately, the three steady-state P/R models developed for the coupled steady-state Exercise III-1 were utilized as the starting point for various sets of 1,000 CRW transients. The results obtained for both 2 and 8-group versions of the models were also compared to assess the impact of the energy-group structure on the main FOMs: total reactor power and MFT.

The trends identified for coupled steady-state total power and MFT mean and standard deviations were also confirmed for the CRW transient, and the main sensitivity drivers were also found to be the same. The choice of energy groups has a significantly larger impact on the mean local power (14.6%) than the mean local fuel temperatures (3.1%), but the standard deviations were less affected by the energy-group choice (0.1–0.7%). The 2-group model mostly overestimated the mean local-power generation but underestimated the local mean fuel temperatures in large areas of the core and should only be used for early scoping studies, where these approximations to the mean values can be tolerated.

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For estimates of the standard deviations in the power and fuel temperatures, a 2-group structure can still be utilized, but the inclusion of TF input uncertainties is essential, especially for local PP estimates. This conclusion is again similar to earlier conclusions reached for Exercise II-2 in Section 6.2.2 and Exercise III-1 in Section 8.1.4, and remains an important contribution of this work to HTGR U/SA.

In terms of the sensitivities of input uncertainties, it was again observed that uncertainties in the model boundary conditions (or total operational measurements) produced the largest sensitivities. Further improvements in the assessment of the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction are also recommended to reduce the uncertainty of the CRW simulation results because this reaction produced the largest sensitivity coefficient of all propagated nuclear data uncertainties. The sensitivity coefficients obtained for uncertainties in material properties (e.g. reflector and fuel graphite thermal conductivity) seem to be much less important than uncertainties in the boundary conditions and the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  reaction.

## 9. CONCLUSIONS

*"Before I came here, I was confused about this subject. Having listened to your lecture I am still confused. But on a higher level." Enrico Fermi.*

The main objective of the research presented in this dissertation was the development of a consistent and effective statistical uncertainty and sensitivity assessment methodology for prismatic<sup>65</sup> HTGRs. This contribution was primarily motivated by the lack of operational and experimental V&V HTGR data and the need to include non-linear coupled phenomena (e.g., coolant core bypass flows). Additional major contributions include the development of a series of benchmark exercises based on the GA MHTGR-350 design that covers both the multi-scale (unit cell, lattice and core) and multi-physics (coupled neutronics and thermal fluids) simulation of a prismatic HTGR, and was formally accepted as part of the IAEA CRP on HTR UAM.

The contributions, main results and conclusions obtained as part of this study are summarized in Section 9.1, followed by recommendations for future research in Section 9.2.

### 9.1 Summary

The summary of the work performed for the research reported in this dissertation is based on the research objectives and contributions identified in Section 1.2.

#### 9.1.1 Development of Prismatic HTGR U/SA Benchmark Specifications.

The first objective of this research was the establishment of a benchmark specification for the uncertainty and sensitivity assessment of a prismatic HTGR that has multi-scale (cell, lattice and core), multiphysics (neutronics, thermal fluids) and safety case applications (normal operation steady-state and off-normal transient conditions). The development of a HTGR U/SA benchmark, and specifically the definition of the Phase II-IV core exercises, was performed as part of the authors' contributions to the IAEA CRP on HTGR UAM as the U.S. DOE representative. The purpose of the benchmark is to provide a reference set of prismatic HTGR specifications that can be used by HTGR developers, nuclear regulators and academia to verify uncertainty assessment methods and codes that is currently being developed.

The prismatic benchmark exercises specified in the various sections of this dissertation are based on the phased approach followed by the OECD/NEA LWR UAM benchmark, consisting of propagating input uncertainties in nuclear data, thermal fluids and reactor operating conditions through the typical LWR core simulation sequence (cell, lattice, core).

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<sup>65</sup> It is indicated in Section 9.2 that the U/SA methodology can also be applied to pebble bed HTGRs without modification.

A decision was taken early in the benchmark development to define the prismatic HTGR neutronics “lattice cell” unit as either a single fuel block or a collection of a central fuel blocks and its six immediate neighbours in an effort to account for the impact of the spectral environment during the cross-section generation process.

In addition to leading the development of the Phase I and stand-alone core exercises (II-1 and II-2), the author’s unique contributions in this area are the development of the Exercise II-4 thermal fluid specifications (Section 7.1), the coupled steady-state exercise III-1 (Section 8.1.1), and the two coupled transients exercises (exercise IV-1 in Section 7.5; exercise IV-2 in Section 8.2.1). The MHTGR-350 design was chosen as the reference reactor design since an existing best-estimate benchmark was already in progress under OECD/NEA guidance (the author was also involved in this earlier benchmark development). In addition to compiling the reactor geometry, material specifications and operating conditions into a cohesive set of specifications, a significant effort was spent on including uncertainty data on fuel, reflector and structural material properties (density, conductivity, etc.), reactor operational conditions and bypass flows into the benchmark specifications.

### **9.1.2 Development of a Consistent and Effective Statistical Uncertainty/Sensitivity Assessment Methodology.**

The primary contribution of this research is the development of a consistent and flexible statistical U/SA methodology and its application to the IAEA CRP on HTGR UAM set of exercises. The statistical methodology consists of a phased approach where cross-section and thermal fluid input uncertainties are assessed independently for lattice and full core calculations, and eventually combined for integral coupled steady-state and transient analysis. This approach allows HTGR core designers and regulators to firstly isolate the impacts of uncertainties in neutronics and thermal fluid input parameters in stand-alone models, followed by the combination of all uncertainties in a consistent and time-dependent coupled model that inherently captures non-linear and feedback effects. The objective of applying this U/SA methodology is to provide increased robustness in the analysis and reactor design process, in addition to providing estimates of available safety margins and data for HTGR BEPU licensing.

In contrast to LWRs, the uncertainty assessment of HTGRs has specific challenges that do not currently allow implementation of a deterministic method. The selection of the statistical methodology is primarily motivated by the lack of HTGR experimental and operational data that is required for deterministic methods.

The second major consideration is the degree to which non-linear dependencies of HTGR thermal fluid parameters could be captured. Adjoint solutions for the dimensional changes of graphite bypass flow channels as a function of irradiation fluence and temperature might be very difficult to obtain as required for deterministic U/SA methods, in contrast to the inclusion of implicit effects in the statistical methodology (e.g., TRISO self-shielding effect during cross-section preparation, or integrated total decay heat from important precursors during the PLOFC).

The use of the statistical U/SA methodology as such is not new (e.g., Bostelmann (2020) also used the SCALE/XSUSA/Sampler approach for the assessment of SFR cross-section uncertainties, and Hernández-Solís (2012) applied a simplified statistical method to LWR cross-section and thermal-hydraulic uncertainties), but the application of a consistent propagated approach to the analysis of coupled HTGR transients is novel. The inclusion of bypass flows as a contributor to overall fuel temperature uncertainty is likewise a unique contribution.

For this research the implementation of the proposed statistical U/SA methodology was demonstrated using existing reactor simulation codes available at INL (SCALE 6.2, PHISICS and RELAP5-3D). These codes were utilized without the need for source code modifications, which is one of the advantages of the proposed methodology (deterministic methods would require development and coding of adjoint solutions in both neutronics and thermal fluid codes). Moreover, the proposed methodology is flexible in the sense that the codes used in this work can be replaced by higher fidelity codes such tools such as MAMMOTH and Pronghorn to improve the best-estimate baseline results, as long as the cross-section covariance data is propagated consistently to the coupled core models.

### **9.1.3 Application of the Proposed U/SA Methodology to the MHTGR-350 Design.**

As an application demonstration of the proposed U/SA methodology on a prismatic HTGR, the SCALE 6.2, PHISICS and RELAP5-3D codes were selected to assess the uncertainties and primary sensitivity drivers of a few important FOMs (eigenvalue, peak power and maximum fuel temperature). The nominal and U/SA results obtained for the Phase I single block and supercell lattice exercises were reported in Section 5.2. This chapter was the starting point for the primary focus of this work (the Phase III and IV transient core exercises), and detailed the generation of the 252-group perturbed AMPX cross-sections libraries that were used to create the 2,8 and 26-group PHISCS models described in Section 6.2.1.

The RAVEN code was subsequently used to determine the energy-dependent sensitivity and Pearson Correlation coefficients, based on a NEWT/Sampler sample size of 1,000 perturbations each for the fresh (Ex. I-2a), burned (Ex. I-2b) and supercell (Ex. I-2c) models.

## CHAPTER 9: CONCLUSIONS

It was found that the eigenvalue ( $k_{\infty}$ ) relative standard deviations due to the cross-section covariance data varied between 0.50–0.54% for the three lattice models (Table 5-4). The largest nuclide covariance-matrix contributors to the uncertainty in  $k_{\infty}$  for Ex. I-2a were uncertainties in  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  and  $^{238}\text{U}(n,\gamma) / ^{238}\text{U}(n,\gamma)$  reactions, while the capture and fission reactions from the resonance absorber  $^{239}\text{Pu}$  also had significant impact on  $k_{\infty}$  for Ex. I-2b. The uncertainty in the average number of neutrons produced per fission ( $^{235}\text{U}(\bar{\nu})$ ) consistently lead to  $1\sigma$  standard deviations of approximately 0.5% across all the fresh and mixed MHTGR-350 lattice and core models used in this research, and dominated any of the other nuclear data uncertainties included in Sampler. This observation leads to the first major recommendation: if any future improvements in measured ENDF data is planned, priority should be given to minimize the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  covariance as far as possible.

For the Phase II core models, cross-section uncertainties from the Phase I lattice models were propagated to the Ex. II-2a and II-2b PHISICS stand-alone neutronics core models as 8-and 26-group perturbed cross-section libraries (Section 6.2). The uncertainties observed for the fresh and mixed-core Phase II models (0.44-0.51%) were found to be similar to the uncertainties calculated for the Phase I lattice models (0.50–0.54%), indicating that the propagation of the 252-group NEWT/Sampler cross-section covariance data into the 26-group PHISICS model preserved the implicit uncertainty information within the 1,000 perturbed libraries. It was also found that the 26- and 8-group eigenvalue standard-deviation results (0.44–0.51% eight fresh and mixed core variants) were almost identical. It was concluded that the additional expense of performing a large number of statistical perturbations using more than eight groups for U/SA purposes is not justified. Since most reactor simulation codes' computational cost will scale directly with the number of energy groups, this conclusion could be a useful to HTGR developers during the earlier stages of design when larger uncertainty margins in best-estimate predictions can be tolerated.

In addition, it was found that the use of larger lattice supercells to generate cross-sections for the peripheral core blocks had a significant effect on the mean eigenvalues, confirming the importance of the softer spectral environment in these peripheral regions for nominal best-estimate calculations. However, in contrast to this trend, it was observed that the impact of the supercells on the  $k_{\text{eff}}$  uncertainties were insignificant, leading to the important conclusion that the impact of cross-section data uncertainties is mostly insensitive to the spectral environment.

In practice this implies that simpler and computationally less-expensive lattice models (single fuel blocks) can be utilized by prismatic HTGR core designers if the main purpose of the model is uncertainty and sensitivity assessment.

## CHAPTER 9: CONCLUSIONS

The first application of the statistical-sampling methodology on prismatic HTGR core thermal fluids simulations was presented in Sections 7.4 and 7.5 for the Ex. II-4 stand-alone thermal fluids steady state and Ex. IV-1 PLOFC transient cases, respectively. A specific focus of this chapter was the uncertainty assessment of bypass flows, where it was found that the addition of bypass flows to the RELAP5-3D model resulted in significantly higher mean fuel temperatures (up to 5.2%), but the fuel temperature uncertainty ( $1\sigma$ ) only varied between 0.7% and 0.9% from the top to the bottom of the core. It was concluded that the inclusion of bypass flows and their uncertainties in the steady-state MHTGR-350 model had no impact on fuel-temperature uncertainties. This finding is again of practical worth to HTGR core designers, since it implies that simpler core models without bypass flow uncertainties can be used for uncertainty assessments. In terms of the main sensitivity drivers, it was found that regardless of the inclusion of bypass flows in the models, the highest-ranked parameters were uncertainties in the three operational boundary conditions: total power, inlet mass-flow rate, and inlet-gas temperature. The impact of uncertainties in the Graphite H-451 thermal conductivity on the maximum fuel temperature was ranked fourth.

The PLOFC transient subsequently utilized the Ex. II-4 perturbed stand-alone RELAP5-3D thermal fluid models as the starting point of the event. It was reported in Section 7.5 that the MFT  $1\sigma$  uncertainty ranged between 0.9-1.8% over the duration of the transient, which was larger than the steady-state uncertainty range due to the addition of decay-heat uncertainties. During the first three hours, the three dominant steady-state boundary-condition parameters retained their respective sensitivity coefficient rankings, but the impact of decay-heat uncertainties surpassed all other input uncertainties after approximately three hours.

For the Ex. III-1 coupled neutronics/thermal fluid model, the main objective was the combined uncertainty assessment of both neutronics and thermal fluids input uncertainties. It was found that although the power distribution and control-rod worths were affected more significantly by cross-section uncertainties, the convective heat transfer via forced helium gas flow minimized the impact of these variations on the fuel temperatures. Local power density  $1\sigma$  uncertainties up to 3.6% were observed in the colder regions of the core, while the local maximum fuel temperature uncertainties reached 1.5% for the models that included thermal fluid uncertainties.

The inclusion of cross-section uncertainties had a smaller impact on the fuel temperature than the inclusion of thermal fluid input parameters. The cross-section uncertainties produced a 0.2–2.0% standard deviation in the local power, but the addition of thermal fluid uncertainties caused significantly higher standard deviations (2.0–3.6%); especially in the upper region of the core where the peak power occurs.

## CHAPTER 9: CONCLUSIONS

These uncertainties in local power and fuel temperature are significant enough to take into account during the design-margin assessment process, but it is much lower than the historic values assumed by GA of up to 15% in fuel temperatures and 10% in local power (Baxter, 2010). The value of the BEPU approach vs. very conservative assumptions is therefore illustrated by this comparison.

As was observed for the PLOFC transient, the main contributors to uncertainties in the Ex. III-1 steady-state power density and fuel temperatures were likewise uncertainties in the reactor operating conditions (total power, inlet mass flow rate and inlet gas temperature). It is therefore recommended that improvements in mass flow, power and gas temperature measurement uncertainties would contribute the most to decrease the overall power density and fuel temperature uncertainties, and should be the focus for directing future margin enhancement and uncertainty reduction efforts. Variations in the bypass flows did not have significant impact on any of the output variables, and for the nuclear data uncertainties it was confirmed that the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  covariance again produced the largest sensitivity in terms of its impact on both the eigenvalue and peak reactor power.

In terms of the energy group structure impact, the use of eight or more energy groups is still recommended for best-estimate HTGR simulation, but in terms of U/SA, two-group models also produced acceptable results for the maximum fuel temperature. However, if the target FOM is the local power peaking, it was shown that eight or more energy groups that are optimized to capture the physics of the  $^{238}\text{U}(n,\gamma)$  and  $^{239}\text{Pu}(n,\gamma)$  resonance regions would be required for accurate uncertainty assessments.

The Ex. IV-2 CRW transient was used in Section 8.2 as an example of a coupled neutronics and thermal fluid simulation that is required as part of a typical HTGR safety case, and concluded the propagation of the SCALE/Sampler cross-section uncertainties from the Phase I lattice to the coupled full-core Phase IV. The trends identified for the Ex. III-1 coupled steady-state total power and fuel temperature mean and standard deviations were very similar for the CRW transient, and the main sensitivity drivers were also found to be the same. The choice of energy groups has a significantly larger impact on the mean local power (14.6%) than the mean local fuel temperatures (3.1%), but the uncertainties in these parameters (standard deviations) were much less affected by the energy-group choice (0.1–0.7%). It was furthermore confirmed that the sensitivity coefficients obtained for uncertainties in material properties (e.g. reflector and fuel graphite thermal conductivity) seem to be much less important than uncertainties in the boundary conditions and the  $^{235}\text{U}(\bar{v}) / ^{235}\text{U}(\bar{v})$  reaction.

#### 9.1.4 Validation of the Proposed U/SA Methodology Against Experimental VHTRC Data.

As the final contribution of this research to the HTGR uncertainty assessment domain, the proposed statistical U/SA methodology was applied in Chapter 4 to a series of temperature-dependent criticality data measured at the experimental VHTRC facility as a partial validation of the Sampler, NEWT, PHISICS and RAVEN sequence utilized for the MHTGR-350 design in Chapters 5-8. Because there is currently very limited measured data available on thermal fluid uncertainties for experimental separate-effects and integral facilities, this validation effort was only focused on uncertainties in neutronics parameters. The VHTRC experimental uncertainties require careful interpretation, since the benchmark team used a mixture of both measured and calculated uncertainty components to derive the final experimental uncertainties. The uncertainty and sensitivity contributors for two critical VHTRC core configurations at five temperatures were compared using the TSUNAMI, Sampler and PHISICS/RAVEN sequences for both the 8- and 26-group models.

It was found that the 26-group NEWT results matched the experimental data significantly better than the 8-group data, but for the assessment of cross-section uncertainties, the 8- and 26-group structures produced identical eigenvalue uncertainties. The calculated PHISICS and experimental mean eigenvalues agreed within  $2\sigma$  of the experimental uncertainty, which was deemed as acceptable within the context of the various assumptions made during the development of the models. The use of the 8-group structure in Chapter 8 for the U/SA of the MHTGR-350 transients could therefore be justified if best-estimate nominal values are not the focus.

The main observation was that regardless of the VHTRC-core loading and temperature, the uncertainties in the cross-sections led to PHISICS eigenvalue uncertainties of approximately 0.64%. These uncertainty results were very well matched with the Sampler/KENO-VI and TSUNAMI model predictions of 0.66%, as well as the benchmark experimental uncertainty data set. Because the NEWT and KENO-VI models were independently developed, and both statistical (Sampler) and deterministic (TSUNAMI) methods were used, it was concluded that the VHTRC data set and the degree of agreement obtained provided a very good verification basis for the use of the Sampler/NEWT/PHISICS sequence selected for this research work.

Furthermore, a comparison of the work performed by Rouxelin (2019) using the same Sampler, NEWT and PHISICS models on the impact of manufacturing uncertainties led to the conclusion that the cross-section uncertainties lead to larger uncertainties in the VHTRC eigenvalue (631–654 pcm) than manufacturing uncertainties (233–346 pcm); a finding confirmed in other studies as well (see Section 9.2).

In terms of the sensitivity analysis, roughly similar trends were observed between the Sampler/RAVEN and TSUNAMI results, with the  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$ , C-graphite (n,n') / C-graphite (n,n') reactions producing the highest ranked sensitivity coefficients. As noted in the MHTGR-350 summary section above, the uncertainty in  $^{235}\text{U}(\bar{\nu})$  was again identified as the most important covariance reaction that should be the focus of future nuclear data improvement efforts.

## 9.2 Recommendations for Future Work

The research reported in this work focused on the assessment of uncertainties in the nuclear cross-section data and a subset of reactor operational conditions and material properties. The five aspects listed below are therefore recommended for further research.

### 9.2.1 Assessment of Additional Input Uncertainties

The focus of this dissertation is primarily on the propagation of uncertainties in the nuclear cross-sections and a subset of thermal fluid parameters across multiple spatial scales and physics. The impacts of uncertainties in material properties (e.g., TRISO radii, densities of TRISO layers and graphite) and fuel manufacturing data (e.g., the number of fuel kernels per compact) were excluded from the scope of the current research. Although material property uncertainties were reported in other applications to be of secondary importance to cross-section uncertainties (e.g., Kim, et al., 2018 reported that the HTGR pebble bed eigenvalue uncertainty contributions due to manufacturing and cross-section input were calculated as 147 pcm and 707 pcm, respectively), it should nevertheless be combined with the other sources of the total simulation uncertainty as part of a comprehensive study.

It was furthermore noted in Section 8.2.1 that the transient results presented for the CRW event did not include the assessment of uncertainties in kinetic parameters (delayed neutron yields and  $\beta_{\text{eff}}$ ), primarily due to the current lack of good quality information on these uncertainties. It is expected that the updated version of SCALE 6.3 that will be released later in 2020 will include these uncertainties in the nuclear covariance data files, which implies that this uncertainty can easily be integrated in the current Sampler stochastic sequence without additional modifications.

### **9.2.2 Use of High-Fidelity Best-Estimate Simulation Codes to Assess Model Uncertainties**

As an example of an application of the proposed HTGR U/SA methodology, the results presented in this work are based on a specific PHISICS/RELAP5-3D model of the MHTGR-350 design. Since the homogenized “ring” model can for example not be used to calculate power and temperature peaking on a block-by-block level, codes like the INL tools MAMMOTH (Ortensi et al., 2018) and Pronghorn (Zou et al., 2017) could be used to assess the impacts of uncertainties in the different physical models and homogenization schemes utilized, and confirm that the general best-estimate and U/SA trends and conclusions made in this work are still valid. The DAKOTA (Adams et al., 2016) U/SA code could also be used in the place of RAVEN to confirm the statistical results obtained. One of the main objectives of this work was the development of a flexible U/SA methodology that could be applied to any new reactor codes capable of simulation HTGRs, without requiring source code modification to the neutronic or thermal fluid solvers. By testing various combinations of high and lower fidelity simulation codes, the independent issue of model and code uncertainties can be assessed as part of HTGR design margin assessment.

### **9.2.3 Extension of Sensitivity Assessment to Identify Individual Contributions to Total Uncertainty (Sensitivity Indices)**

The sensitivity analysis performed as part of this work was limited to the current capabilities of the RAVEN code, and a secondary focus to the overall uncertainty assessment effort. The sensitivity coefficients obtained are simple linear coefficients that indicate how much the FOM will change for a change in the parameter, but as noted in several sections in this dissertation, the specific contribution of a parameter to the total uncertainty in the FOM cannot be determined with this approach.

A notable improvement on the current approach will therefore be the implementation of variance-based sensitivity indicators like Sobol’s first order and total indices (Sobol, 2001), or rather variance-based indices based on linear perturbation theory, as suggested by Bostelmann (2020). In her Ph.D. dissertation research on the U/SA of SFR systems, Bostelmann implemented and compared three different sensitivity indices, and a similar effort for HTGRs would enable the determination of sensitivity contribution indicators to the total power density and fuel temperature uncertainties (for example). It should however be noted that Bostelmann’s implementation was limited to neutronic parameters; the development and calculation effort required to extend her work to the coupled thermal fluid and neutronics transient domain might be considerable.

#### 9.2.4 Availability of New Validation Data

A major motivation for the choice of the statistical U/SA methodology for HTGRs is the lack of experimental and operational V&V data. If additional V&V data becomes available, e.g. through the planned 2021 restart of the Japanese HTTR LOFC experiments or the first-critical core start-up of the HTR-PM in China in 2020 (for pebble bed reactors), data from these facilities can possibly be used as validation benchmarks for the statistical methodology, or to develop variance-based deterministic U/SA methods that can be compared with the results obtained with the statistical approach utilized in this work.

#### 9.2.5 Extension of the Proposed Methodology to Pebble Bed HTRs and Beyond Core Simulation

It is expected that the same statistical U/SA methodology presented in this research could be applied to coupled transient analysis of gas and molten salt cooled pebble bed HTRs, but confirmatory studies using similar stochastic schemes would be required to confirm this expectation. In terms of pebble bed-specific phenomena, the continuous movement, depletion and reloading of pebble fuel could add additional uncertainty elements that were not considered in this work for the prismatic MHTGR-350. Hao et al. (2015) specifically investigated the impact of uncertainties in the pebble bed filling fraction, while Cheng et al. (2020) reported the uncertainty results obtained for various TRISO lattice or random representation models within the pebble fuel. A recent paper by Hao et al. (2020) reports the U/SA results of a DLOFC event for the HTR-PM performed with the newly developed Advanced Thermal-Hydraulic Energy Network Analyser (ATHENA) and Code of Uncertainty and Sensitivity Analysis (CUSA) codes, but it seems this work was limited to the perturbation of thermal fluid parameters only.

Moreover, the statistical methodology described in the current work can in principle also be applied to assess uncertainties and sensitivities in fuel performance, fission product release and worker/public dose calculations. The propagation of cross-section and thermal fluid uncertainties as perturbed primary system models can for example be used as input to fuel performance codes like BISON (Hales, et al. (2013)) and PANAMA (Verfondern, 2014) for a complete uncertainty assessment of the fuel-to-vessel-to-building source term.

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## Appendix A: MHTGR-350 Design

A summarized overview of the 350 MWt MHTGR design and the benchmark specifications based on this design is provided in this appendix. The MHTGR-350 is a prismatic HTGR design that was developed (but never built) by GA in the 1980s. It was chosen as the reference design for the OECD/NEA MHTGR-350 benchmark (OECD/NEA, 2018) because detailed design and safety information is publicly available from the Preliminary Safety Information Document (Stone and Webster Engineering Corporation 1986) that was submitted to the U.S. NRC. A subsequent review of the MHTGR licensing basis accident scenarios was performed by Brookhaven National Laboratory (BNL) for the NRC (Kroeger 1989), and draft licensing review report by published by the NRC (Williams et al. 1989).

It is important to note that although the same geometrical and operational reactor-design information is used for both the OECD/NEA MHTGR-350 and IAEA CRP HTGR UAM benchmarks, the definition of the core states differs significantly. For the OECD/NEA MHTGR-350 benchmark, additional non-public end of equilibrium cycle nuclide data was provided by GA to the INL benchmark team. A fresh-core case was not defined, and the mixed core consisted of 220 fuel blocks that had been shuffled and reloaded after one and two burn cycles, respectively. Each of the 220 fuel blocks (22 fuel blocks in 10 axial layers) had a unique nuclide composition; therefore, cross-section libraries, based on their specific exposure histories.

In contrast to this, the IAEA CRP on HTGR UAM simplified this approach by specifying a fresh core that consists only of fresh fuel everywhere for Exercise II-2a (i.e. a single cross-section and isotopic data set), as well as a mixed core that contains fresh and depleted fuel blocks (Exercise II-2b) in ten identical axial core layers. Although the mixed-core packing pattern is the same for both benchmarks, the depletion state of the burned blocks is not the same. This essentially decoupled the CRP models from the non-public GA data set and allowed participants to build the fresh and depleted core cross-sections and propagate the covariance uncertainty data, using their own lattice tools. However, this means that direct comparisons of eigenvalues, power densities, and temperatures between the two benchmarks are not possible. This approach is judged to be acceptable because the primary purpose of the IAEA CRP on HTGR UAM is a comparison of uncertainty and sensitivity parameters, not best-estimate/nominal values of the “as-designed” MHTGR-350.

The information provided in this Appendix is based on the first official release of the OECD/NEA MHTGR-350 benchmark specification (OECD/NEA 2018). The main characteristics of the MHTGR-350 design is summarized in Table A-1.

Table A-1. MHTGR-350 core-design parameters.

| Core Parameter                               | Value                                                                                                                |
|----------------------------------------------|----------------------------------------------------------------------------------------------------------------------|
| Number of fuel columns                       | 66                                                                                                                   |
| Installed thermal/electrical capacity        | 350 MWt /165 MWe                                                                                                     |
| Core configuration                           | Annular                                                                                                              |
| Fuel                                         | Prismatic Hex-Block fueled with uranium oxycarbide fuel compact of 15.5 weight % enriched $^{235}\text{U}$ (average) |
| Primary coolant                              | Helium                                                                                                               |
| Primary coolant pressure                     | 6.39 MPa                                                                                                             |
| Moderator                                    | Graphite                                                                                                             |
| Core-outlet temperature                      | 687°C                                                                                                                |
| Core inlet temperature                       | 259°C                                                                                                                |
| Mass-Flow Rate                               | 157.1 kg/s                                                                                                           |
| Reactor-Vessel Height                        | 22 m                                                                                                                 |
| Reactor-Vessel Outside Diameter              | 6.8 m                                                                                                                |
| Effective inner diameter of active core      | 1.65 m                                                                                                               |
| Effective outer diameter of active core      | 3.5 m                                                                                                                |
| Active-core height                           | 7.93 m                                                                                                               |
| Number of standard/RSC fuel elements         | 540 / 120                                                                                                            |
| Number of inner/outer reflector control rods | 6 / 24                                                                                                               |
| Number of RSC channels in core               | 12                                                                                                                   |

The RPV contains the reactor core, reflectors, and associated neutron-control systems, core-support structures, and shutdown cooling heat exchanger and motor-driven circulator. The RPV is uninsulated to provide for decay-heat removal under loss-of-forced-circulation conditions. In such events, heat is transported to the passive Reactor Cavity Cooling System (RCCS), which circulates outside air by natural circulation within enclosed panels surrounding the RPV. The core is designed to provide 350 MWt at an average power density of  $5.9 \text{ MW/m}^3$ . A core elevation view is shown in Figure A-1, and a plane view is shown in Figure A-2.

The design of the core consists of an array of hexagonal fuel elements in a cylindrical arrangement surrounded by a single ring of identically sized solid-graphite replaceable reflector elements, followed by a region of permanent reflector elements, all located within a RPV. The fuel elements are stacked to form columns (10 fuel elements per column) that rest on support structures. The active-core columns form a three-row annulus, with columns of hexagonal graphite reflector elements in the inner and outer regions. Thirty reflector columns contain channels for control rods, and 12 columns in the core also contain channels for the reserve shutdown material. The active-core effective outer diameter of 3.5 m is sized to maintain a minimum reflector thickness of 1 m within the 6.55 m inner diameter reactor vessel. The height of the core with ten elements in each column is 7.9 m.

Core reactivity is controlled by a combination of LBP, movable poison, and a negative temperature coefficient. This fixed poison is in the form of LBP compacts; the movable poison is in the form of metal-clad control rods. The fuel comprises of (TRISO) fuel particles bonded in a graphite matrix to form a cylindrical compact. The compacts are then inserted into hexagonal graphite blocks to construct a fuel element. More detail on the core radial and axial geometry, fuel, reflector, and control-rod design can be found in the benchmark specification.

Figure A-3 shows the whole core region numbering for the one third core. The bottom reflector is defined as layer 1. Radially, the central column is Column 1, and the rest of the numbering follows the various radial rings up to 91 columns. This numbering system is used for both the IAEA CRP and OECD/NEA benchmarks. The mixed-core fuel-loading pattern is shown in Figure A-4.

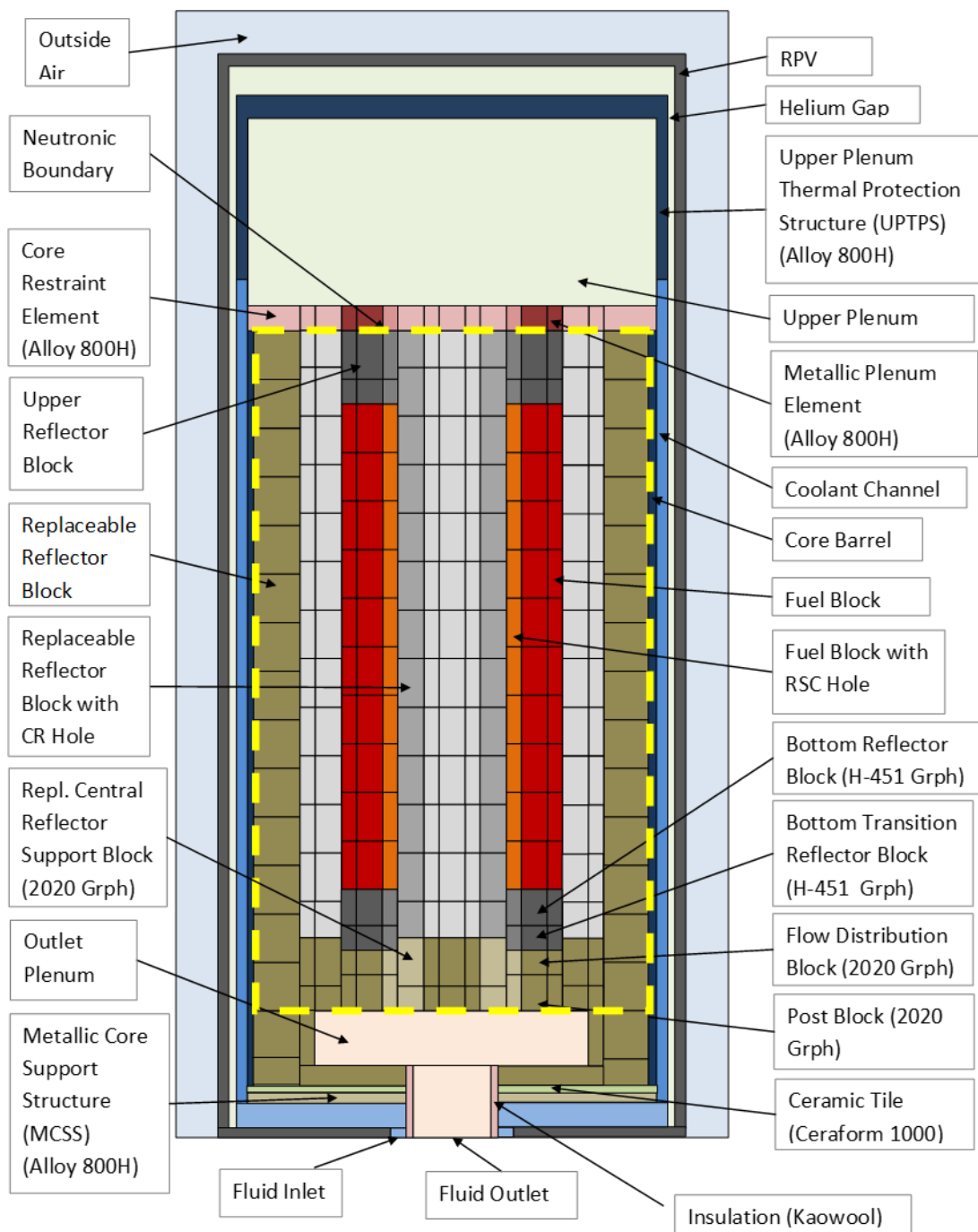


Figure A-1. MHTGR axial layout.

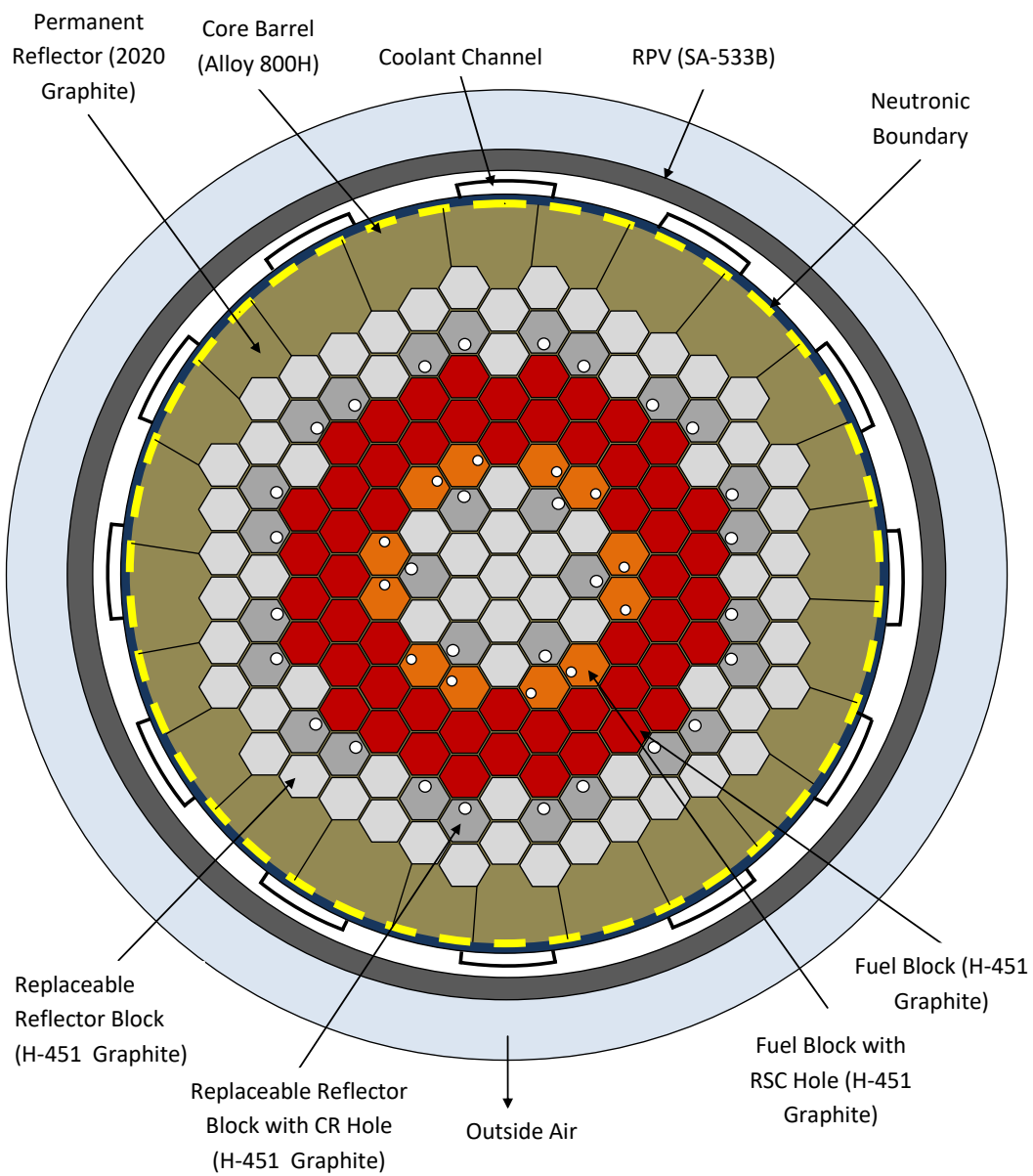


Figure A-2. MHTGR radial layout.

Table A-2. Fuel Element Description.

| Fuel Element Geometry                             | Value                  |
|---------------------------------------------------|------------------------|
| Block-graphite density (for lattice calculations) | 1.85 g/cm <sup>3</sup> |
| Fuel holes per element                            | —                      |
| Standard element                                  | 210                    |
| RSC element                                       | 186                    |
| Fuel hole radius                                  | 0.635 cm               |
| Coolant holes per element (large/small)           | —                      |
| Standard element                                  | 102 / 6                |
| RSC element                                       | 88 / 7                 |
| Large/small coolant hole radius                   | 0.794/0.635 cm         |
| Fuel/coolant pitch                                | 1.8796 cm              |
| Block pitch                                       | 36 cm                  |
| Element length                                    | 79.3 cm                |
| RSC hole diameter                                 | 9.525 cm               |
| LBP holes per element                             | 6                      |
| LBP radius / gap radius                           | 0.5715 cm / 0.635 cm   |

Table A-3. TRISO/fuel compact description.

| TRISO Fuel Element<br>(general design parameters for lattice calculations) | Value                                                                 |
|----------------------------------------------------------------------------|-----------------------------------------------------------------------|
| Fissile material                                                           | UC <sub>0.5</sub> O <sub>1.5</sub>                                    |
| Enrichment ( <sup>235</sup> U average)                                     | 15.5 w/o                                                              |
| UCO Kernel / Buffer Radii                                                  | 212.5 μm / 312.5 μm                                                   |
| IPyC / SiC / OPyC Radii                                                    | 347.5 μm / 382.5 μm / 422.5 μm                                        |
| UCO Kernel / Buffer Densities                                              | 10.5 g/cm <sup>3</sup> / 1.0 g/cm <sup>3</sup>                        |
| IPyC / SiC / OPyC Densities                                                | 1.9 g/cm <sup>3</sup> / 3.2 g/cm <sup>3</sup> / 1.9 g/cm <sup>3</sup> |
| Packing Fraction (average)                                                 | 0.350                                                                 |
| Compact Radius / Length                                                    | 0.6225 cm / 4.928 cm                                                  |
| Compact Gap Radius                                                         | 0.635 cm                                                              |

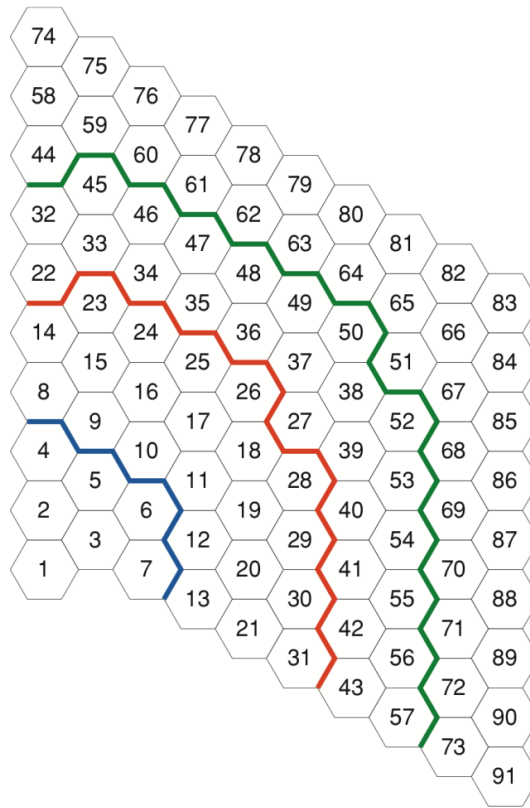


Figure A-3. Whole core-numbering layout (Layer 1).

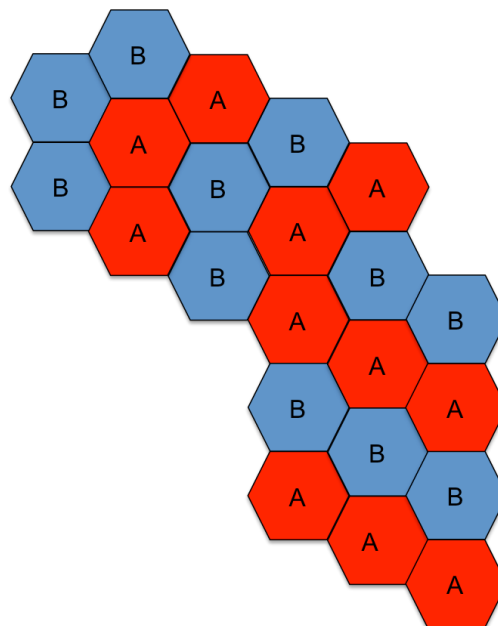


Figure A-4. Mixed-core loading pattern: fresh (A) and depleted (B) fuel.

## Appendix B: Description of Codes and Models

This appendix provides short descriptions of the primary codes and selected models utilized in this research work.

### B-1. PHISICS/RELAP5-3D

The theoretical basis of the coupled PHISICS/RELAP5-3D code is detailed in the 2016 publication of Rabiti, et al.; the summary below is mainly based on the descriptions in this publication. The PHISICS code primarily consists of a time-dependent nodal transport core solver (INSTANT), a depletion module Multi Reactor Transmutation Analysis Utility (MRTAU) and a cross section interpolation routine (Mixer). The INSTANT core solver is based on the second order formulation of the transport equation discretized in angle by spherical harmonics, while it uses orthonormal polynomials of an arbitrary order for the spatial variable. The time discretization of the transport equation is based on an intrinsic stable backward Euler scheme. The MRTAU depletion module calculates time-dependent isotopic changes as a function of the local flux, in addition to natural decay. The code uses a Taylor series expansion-based algorithm of arbitrary order and the Chebyshev Rational Approximation Method for computation of the exponential matrix.

PHISICS was coupled to the RELAP5-3D thermal-hydraulics code as a set of subroutines, giving the user access to the full capability of PHISICS from within RELAP5-3D. As a system thermal-fluid code, RELAP5-3D was initially developed for LWR and BWR analysis (Mesina, 2016), but the inclusion of helium-gas properties also allows the assessment of HTGR systems. RELAP5-3D is primarily used as a primary and secondary system code, and is capable of full three-dimensional hydrodynamics in rectangular, cylindrical, and spherical geometries. It also includes two-dimensional heat transfer simulation via conduction, convection, and radiation – for the MHTGR-350 model, 2D conduction is an important capability that is used extensively.

The PHISICS/RELAP5-3D driver collects geometry and calculation option data from RELAP5-3D in addition to data from the PHISICS input files (i.e. cross-sections, transport solver options, depletion parameters, etc.). The iteration scheme exchanges power density data from PHISICS and fuel/moderator temperatures from RELAP5-3D between the modules until convergence is reached. The general data flow between the modules are shown in Figure B-1, while the coupled steady-state solution scheme is presented in Figure B-2. The interested reader is referred to the publication by Rabiti, et al. (2016) for details on the discretization schemes implemented for all these solvers.

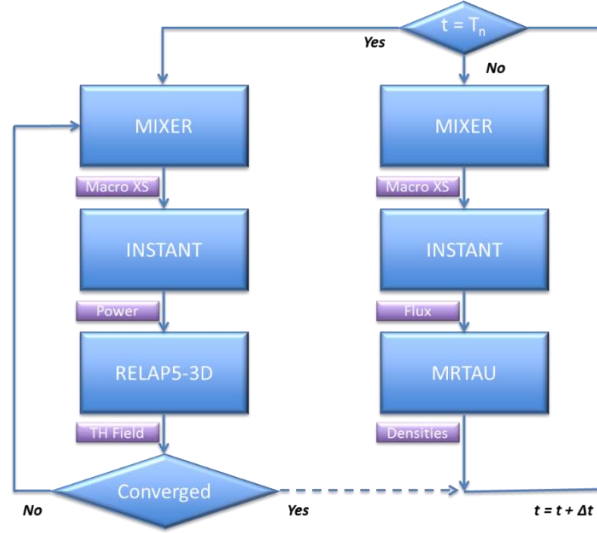


Figure B-1. PHISICS/RELAP-3D data flow (Strydom, et al., 2016).

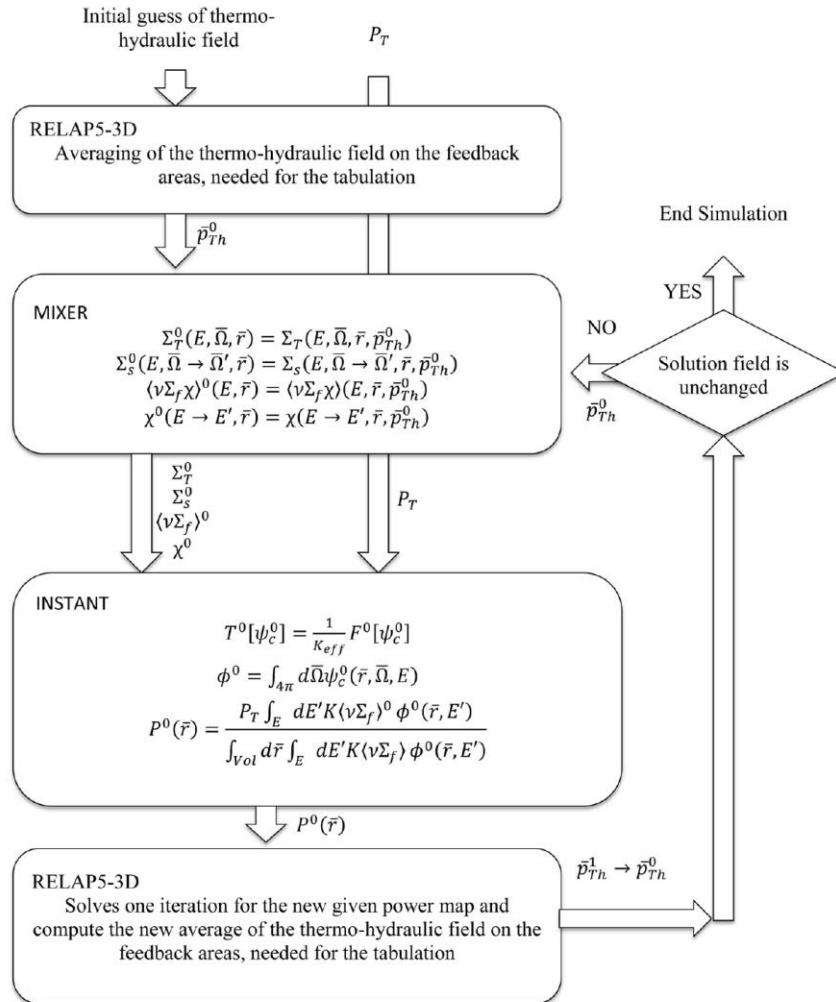


Figure B-2. PHISICS/RELAP5-3D coupled steady-state solution scheme (Rabiti, et al., 2016)

### The RELAP5-3D MHTGR-350 “ring” model

The work reported in this dissertation uses the “ring” version of the MHTGR-350 model developed for the OECD/NEA MHTGR-350 benchmark. A concise description of this model is provided here; for further details, the reader is referred to Strydom, et al. (2016). The ring model follows the common system-code homogenization approach of modelling the inner reflector, fueled core region, and outer reflector as rings in cylindrical coordinates, with three additional rings representing the core barrel, RPV, and outer air boundary layer, as shown in Figure B-3. The radii of the rings are calculated to represent the correct graphite volumes in each of the structures, and it includes corrections for the 2 mm gaps between the reflector blocks and the 3 mm gap between the outer reflector and the metallic core barrel.

In the MHTGR-350 core design, neutronic feedbacks on the fuel and moderator (graphite) temperatures are quite different. Therefore, it is desirable to have an accurate prediction of the fuel and moderator temperatures independently. To model the fuel region of the core, a cylindrical “unit cell” has been defined, consisting of a fuel compact, its surrounding matrix graphite and a helium coolant channel (Figure B-3). In this approach, the fuel compact (TRISO fuel particles embedded in graphite) is homogenization to a single region. The unit cell is constructed as follows:

- The radius of the coolant hole corresponds to the actual design radius.
- The distance between the coolant hole and the homogenized fuel region, i.e. the thickness of the inner graphite region, corresponds to the design distance so that the heat transfer distance is conserved.
- The homogenized fuel region conserves the design fuel volume, i.e. the thickness of this region is determined by the fuel volume in the unit cell.
- The size of the outer graphite region (outer ring in Figure B-3) is such that the total graphite mass in the unit cell is represented.

Three unit cells are used to distinguish between the average fuel and moderator temperature in the inner, center and outer fuel rings. In the context of the RELAP5-3D model, the *fuel* temperature is defined as the homogenized fuel region temperature, while the *moderator* temperature is defined as the homogenized temperature of the graphite volume in each of the fuel rings outside the core region. The homogenized graphite temperature for each reflector ring provides the *reflector* temperature feedback reactivity. The core is divided into 14 axial levels, two each for the upper and lower reflector and ten levels for the core region (Figure B-4 right). This leads to a total of 30 fuel temperatures for the active core region (e.g., see Table 7-4). The highest value of this spatial field is designated as the maximum fuel temperature (MFT).

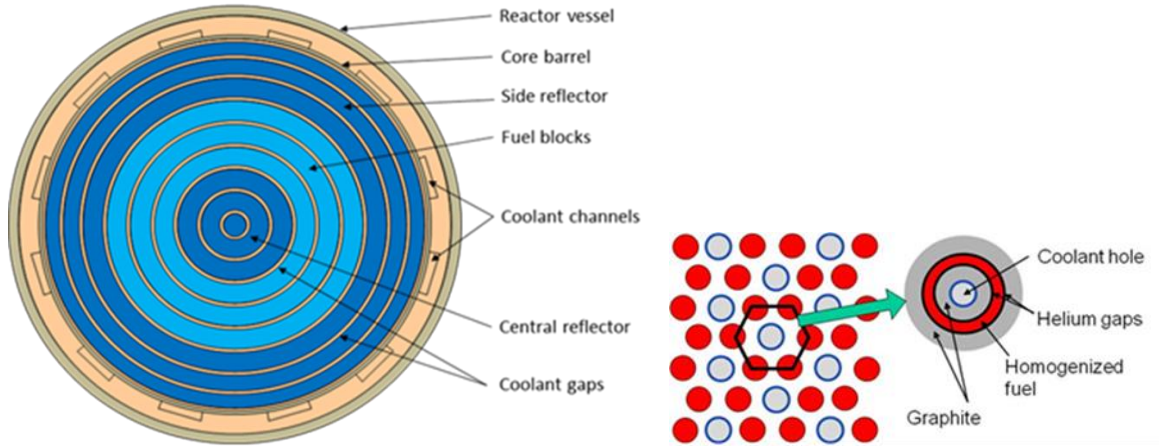


Figure B-3. MHTGR-350 RELAP5-3D “ring” model (left) and fuel unit cell representation (right).

The PHISICS model and coupling with RELAP5-3D is described in Section 6.2.1 and will not be discussed here again. The reactor vessel nodalisation for RELAP5-3D is also shown in Figure B-4. The time-dependent junction #255 adjusts the inflow helium mass flow rate to obtain a target outlet helium temperature of 687°C through a control variable that combines the outlet pressure (6.39 MPa), inlet helium temperature (259°C) and the total thermal power (350 MW) boundary conditions.

In addition to the core region, the model includes the lower plenum (#175), coolant riser (#115), upper plenum (#125), outlet plenum (#170), vessel gap and the vessel metal structures.

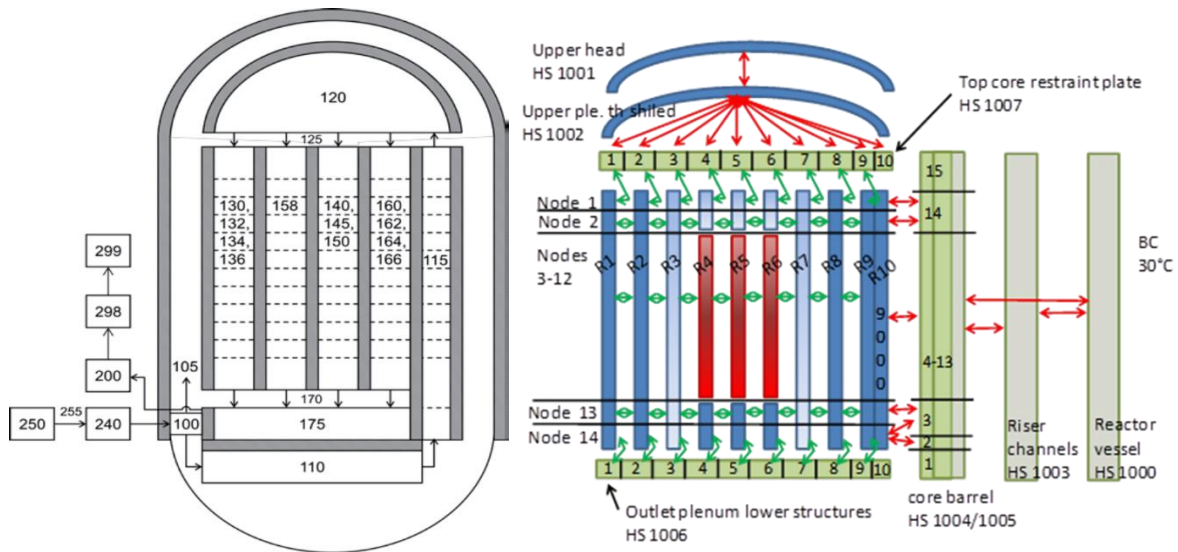


Figure B-4. RELAP5-3D Reactor model nodalisation (left). Conduction (green arrows) and radiation (red arrows) enclosures are shown on the right.

More than 90 conduction and radiation sets are included in the model to account for radial conduction and axial radiation between the graphite structures in the inner, outer, top and bottom reflectors. Radial radiation heat transfer is also modelled between the outer reflector surface and the core barrel, and from the outer surface of the reactor vessel to the boundary air layer, as shown in Figure B-4. Adiabatic boundary conditions are applied at the top and bottom model boundaries, and the outer radial air layer is defined to be at a constant temperature of 30°C.

## **B-2. RAVEN**

RAVEN is a flexible and multi-purpose uncertainty quantification, regression analysis, probabilistic risk assessment, data analysis and model optimization software (Alfonsi, et al. 2017). RAVEN is essentially a “wrapper” code that interfaces with various simulation codes. The user can use RAVEN as the driver code to specify perturbation factors (distribution types, ranges, sampling strategies), create perturbed input decks, perform the perturbed sample set of simulations, and post-process statistical metrics like mean, standard deviations, and sensitivity parameters for the desired FOMs.

The interface between RAVEN and PHISCS/RELAP5-3D was developed by Rouxelin (2019) as part of his Ph.D. work. An interface between RELAP5-3D and RAVEN already existed at that time; Rouxelin added the capability of perturbing additional neutronics PHISICS parameters. In the current work, RAVEN was however not used in this role (i.e. Sampler was used to perturb the cross-sections), but applied to the PHISICS/RELAP5-3D model as described in Section 8.1. to create the perturbed RELAP5-3D input decks for Exercise II-4 and IV-1.

In addition to the Rouxelin’s use of RAVEN to assess the impact of material and manufacturing uncertainties for the VHTRC, the interested reader is referred to previous studies that applied RAVEN to RELAP5-3D assessments of HTGR decay heat surrogate modeling (Alfonsi, et al., 2018), a BWR station blackout (Mandelli, et al., 2016), a molten metal experiment (Narcisi et al., 2019) and the investigation of new cladding criteria for LWRs (Alfonsi, 2017).

RAVEN was also used as the statistical post-processor to calculate the sensitivity parameters (NSC, PCC, mean and standard deviations) discussed in Chapters 4-8. The statistical parameters are listed in the RAVEN User Manual (Alfonsi, et al. 2017). Apart from the conventional definitions of expected (mean) value, standard deviation and variance, the following statically parameters are also used in the discussion of the results (all formulae are from the RAVEN User Manual [Alfonsi, et al. 2017]):

### ***Skewness***

Skewness is a measure of the asymmetry of the distribution of a real-valued random variable about its mean. Negative skewness indicates that the tail on the left side of the distribution is longer than the right side. Skewness is useful to identify the distortion of the random variable with respect to the normal distribution function. It uses the mean ( $\mu$ ) and standard deviation ( $\sigma$ ) and is defined as

$$\gamma_1 = \mathbb{E} \left[ \left( \frac{X - \mu}{\sigma} \right)^3 \right] = \frac{\mathbb{E} [(X - \mu)^3]}{(\mathbb{E} [(X - \mu)^2])^{3/2}}$$

### ***Excess Kurtosis***

Kurtosis indicates the degree of “peakedness” of a distribution of a real-valued random variable. Values greater than zero indicates a peaked distribution; negative values indicate flatter distributions. It is defined as:

$$\gamma_2 = \frac{\mathbb{E} [(X - \mu)^4]}{(\mathbb{E} [(X - \mu)^2])^2}$$

### ***Covariance matrix***

The covariance represents a measurement of the correlation, in terms of variance, among two variables. It is defined as:

$$\Sigma(\mathbf{X}, \mathbf{Y}) = \mathbb{E} \left[ (\mathbf{X} - \mathbb{E}[\mathbf{X}]) (\mathbf{Y} - \mathbb{E}[\mathbf{Y}])^T \right]$$

and is calculated in RAVEN as follows:

$$\mathbb{E} [(X - \mathbb{E}[X]) (Y - \mathbb{E}[Y])] \approx \frac{1}{n} \sum_{i=1}^n (x_i - \mu_x)(y_i - \mu_y)$$

where

- $w_i$  is the weight associated with the sample  $i$  (for the results reported in this work a unit weight of 1.0 is assumed)
- $n$  are the total number of samples
- $V_1 = \sum_{i=1}^n w_i$

### ***Pearson product-moment correlation coefficient (PCC)***

The PCC is defined as the covariance of the two variables divided by the product of their standard deviations:

$$\rho_{XY} = \frac{\text{cov}(X,Y)}{\sigma_X \sigma_Y}$$

and is a measure of linear correlation between variables  $X$  and  $Y$ . The PCC can range between +1 and -1, where 1 is total positive linear correlation, 0 is no correlation, and -1 is total negative linear correlation.

### ***Sensitivity and Normalized Sensitivity coefficients***

RAVEN calculates two sensitivity-coefficient metrics. The first is a matrix of linear-regression sensitivity coefficients that are computed via a least-squares fit routine. It assumes the target value  $y$  can be expressed as a linear combination of the perturbed features  $x_1, x_2, \dots, x_p$  in the format

$$y(w, x) = w_0 + w_1 x_1 + \dots + w_p x_p,$$

with  $w$  the linear-regression sensitivity coefficients. The RAVEN routine fits a linear model with coefficients  $w = (w_1, w_2, \dots, w_p)$  to minimize the residual sum of squares between the observed target values  $y$  and the linear approximation  $y$  values, by solving

$$\min_w \|wx - y\|_2^2$$

For direct comparison between various input parameters, the normalized sensitivity coefficients (NSC) is also used in this work. This is defined in RAVEN as sensitivities normalized with respect to their mean values. These NSCs are useful in the sense that it represent a per-unit sensitivity metric, e.g. in the linear formulation a NSC of -0.5 implies that a perturbation of +1% in the mass-flow rate lead to a decrease of -0.5\*1% = 0.5% in the mean maximum fuel temperature (as discussed in Section 7.5).

## **B-3. SCALE/KENO-VI and SCALE/NEWT**

The SCALE/KENO-VI module was developed at as a three-dimensional Monte Carlo criticality code that utilizes CE or MG ENDF/B-VII.0 or ENDF/B-VII.1 cross-section data (Rearden & Jessee, 2018). The KENO-VI module was only used in this work to provide reference comparison data for the Sampler/NEWT sequence in Chapter 4 and 5. More detail on the MHTGR-350 and VHTRC KENO-VI models used in this work can be found in the publications of Strydom, Bostelmann & Yoon (2015) and Bostelmann and Strydom (2017), respectively.

In CE mode, the double-heterogeneity of a HTGR can be considered by modeling a regular particle lattice that is included in fuel pin, but for MG calculations, problem-dependent cross-sections are determined in a self-shielding calculation prior to the neutron transport calculation. In SCALE version 6.2, material and cross-section processing were modernized and is executed through the Cross (X) Section Processing (XSProc) module.

For MG calculations, XSProc performs the resonance self-shielding, energy group collapse, and spatial homogenization calculations required for the double heterogeneous cells utilized in HTGRs. It should be noted that XSProc sequence is the same regardless of the transport solver selected (KENO-IV or NEWT).

The CENTRM routine within the XSProc module uses two one-dimensional discrete ordinates transport CE calculations to treat the resonance self-shielding of a heterogeneous distribution of TRISO particles within a graphite fuel compact matrix, as shown in Figure B-5. The first CENTRM calculation accounts for the TRISO heterogeneity and is performed on a representative spherical unit cell, consisting of the central UCO fuel kernel and the four surrounding layers; all embedded in a graphite matrix.

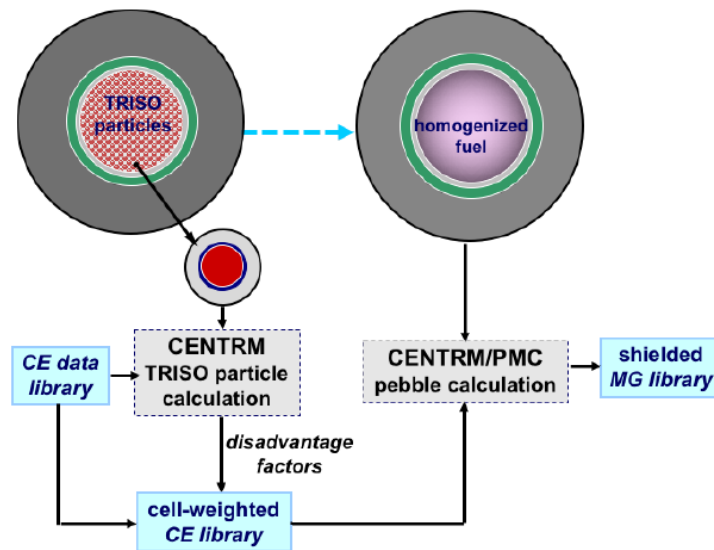


Figure B-5. Overview of double heterogeneous procedure in SCALE 6.2 (Bostelmann, et al., 2018).

This calculation provides a detailed CE flux distribution that are used for the determination of CE disadvantage factors (defined as the ratio of CE flux in the individual zones divided by the cell-averaged CE flux). The disadvantage factors are used to calculate weighted CE cross sections for the homogenized fuel compact in the fuel component. A second CENTRM transport calculation is then performed on a unit cell representing the homogenized fuel component in a representative lattice (Bostelmann, et al., 2018).

For the preparation of HTGR-dependent multigroup cross sections, the TRITON-NEWT (T-NEWT) transport sequence in SCALE builds on the XSProc cross-section processing by automatically executing the 2-D discrete-ordinates transport calculation using the NEWT (New Extended Step Characteristic-based Weighting Transport) code (Rearden & Jessee, 2018). In this study the T-NEWT sequence was used to collapse the 252-group ENDF/B-VII.1 lattice cross-sections to the 2, 8 and 26-group cross-section libraries for use in the PHISICS core calculations.

The flux-weighted collapse is performed to the specified group structure for each nuclide in each material region in the HTGR lattice cell domain, based on the average flux in that material, as shown in Figure 3-5.

## **B-4. SCALE/Sampler and SCALE/TSUNAMI**

Two options are available in SCALE for uncertainty and sensitivity assessment: the deterministic TSUNAMI sequence that utilizes the same T-NEWT sequence as described above with one additional adjoint flux solution step, or the statistical Sampler sequence that does not require an adjoint solution.

In the current research, continuous-energy eigenvalue-sensitivity coefficients were obtained for the VHTRC in Section 4.3.2 with the CE TSUNAMI CLUTCH method (Perfetti et al. 2016). This method allows a more efficient calculation with a smaller computational memory footprint than the Iterated Fission Probability (IFP) eigenvalue-sensitivity method that is also available with CE TSUNAMI. By collapsing the determined sensitivity coefficients with the available covariance data, nuclear data eigenvalue uncertainties were obtained.

Sampler is a statistical “super-sequence” that performs general uncertainty analysis for SCALE sequences by statistically sampling the input data and analyzing the output distributions for specified responses. Random perturbation factors for nuclear cross sections and depletion data are pre-computed with the XSUSA module Medusa by sampling covariance information and are stored in libraries read during the Sampler execution. More detail is provided in Chapter 6 of the SCALE User Manual (Rearden & Jessee, 2018). Sampler was used to generate all the perturbed libraries for the VHTRC and MHTGR-350 models utilised in this work; more detail on the perturbation factors and the calculation sequence can be found in Section 3.2.2.

## Appendix C: Dissertation-Related Publications

During the development of the IAEA CRP on HTGR UAM specifications and subsequent analysis, several peer-reviewed journal and conference publications were completed by the author in a primary or secondary role. A subset of this data set is reported in this dissertation. The references are listed in reverse chronological order in Table C-1.

Table C-1. Author's publications related the IAEA CRP on HTGR UAM (2012-2019).

| Publication                           | Title                                                                                                                                                            | Authors                     | Reference                                             |
|---------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|-------------------------------------------------------|
| <i>Nuclear Engineering and Design</i> | Energy Group Search Engine Based on Surrogate Models Constructed with the NEWT/PHISICS/RAVEN Sequence                                                            | Rouxelin, P. et al.         | <i>Nucl. Eng. Des.</i> 356, 2020.                     |
| <i>Nuclear Engineering and Design</i> | The IAEA CRP on HTGR uncertainties: Sensitivity study of PHISICS/RELAP5-3D MHTGR-350 core calculations using various SCALE/NEWT cross-section sets for Ex. II-1a | Rouxelin, P. et al.         | <i>Nucl. Eng. Des.</i> 329, 2018.                     |
| <i>Annals of Nuclear Energy</i>       | Nuclear data uncertainty and sensitivity analysis of the VHTRC benchmark using SCALE                                                                             | Bostelmann, F., Strydom, G. | <i>Annals of Nuclear Energy</i> 110, 2017.            |
| <i>Nuclear Engineering and Design</i> | The IAEA Coordinated Research program on HTGR Uncertainty Analysis: Phase I status and Ex. I-1 prismatic reference results.                                      | Bostelmann, F. et al.       | <i>Nucl. Eng. Des.</i> 306, 2016.                     |
| <i>Annals of Nuclear Energy</i>       | Criticality calculations of the Very High Temperature Reactor Critical Assembly benchmark with Serpent2 and SCALE/KENO-VI                                        | Bostelmann, F. et al.       | <i>Annals of Nuclear Energy</i> 90, 2016.             |
| HTR 2018 conference                   | IAEA CRP on HTGR UAM: Propagation of Phase I cross-section uncertainties to Phase II neutronics steady-state using SCALE/Sampler and PHISICS/RELAP5-3D           | Strydom, G. et al.          | <i>Proceedings of HTR 2018, Warsaw, Poland, 2018.</i> |
| HTR 2018 conference                   | Decay Heat Surrogate modeling for High Temperature Reactors                                                                                                      | Alfonsi, A. et al.          | <i>Proceedings of HTR 2018, Warsaw, Poland, 2018.</i> |

|                                       |                                                                                                                                                      |                                       |                                                                               |
|---------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------|-------------------------------------------------------------------------------|
| PHYSOR 2018                           | Uncertainty quantification of pebble bed reactor fuels using sampling method: contribution of manufacturing parameters and cross-section uncertainty | Kim, H. et al.                        | <i>Proceedings of PHYSOR 2018, Cancun, Mexico, 2018.</i>                      |
| 2017 American Nuclear Society meeting | IAEA CRP on HTGR uncertainties: quantification of depletion nuclide inventory uncertainties                                                          | Rouxelin, P. et al.                   | <i>Transaction ANS, Winter 2017.</i>                                          |
| PHYSOR 2016 conference                | Quantification of the SCALE 6.1 eigenvalue uncertainty due to cross-section uncertainties for exercise I-1 of the IAEA CRP on HTGR uncertainties     | Naicker, V. et al.                    | <i>ANS topical meeting on reactor physics (PHYSOR 2016), Sun Valley, USA</i>  |
| PHYSOR 2016 conference                | Impact of nuclear data uncertainties on criticality calculations of the Very High Temperature Reactor Critical Assembly Benchmark.                   | Bostelmann, F. et al.                 | <i>ANS topical meeting on reactor physics (PHYSOR 2016), Sun Valley, USA</i>  |
| PHYSOR 2016 conference                | IAEA CRP on HTGR Uncertainties: Comparison of Ex. I-2c Nominal Results and Coupling with the PHISICS/RELAP5-3D Core Model for Ex. II-1               | Rouxelin, P., Strydom, G., Ivanov, K. | <i>ANS topical meeting on reactor physics (PHYSOR 2016), Sun Valley, U.S.</i> |
| ICAPP 2014 conference                 | Comparison of homogeneous and heterogeneous CFD fuel models for Phase I of the IAEA CRP on HTGR uncertainties benchmark                              | Yoon, S-J., Strydom, G.               | <i>Proceedings of ICAPP 2014, Charlotte, USA, 2014.</i>                       |
| HTR 2014 conference                   | The IAEA Coordinated Research program on HTGR Uncertainty Analysis: Phase I status and initial results.                                              | Reitsma, F. et al.                    | <i>Proceedings of HTR 2014, Weihai, China, 2014.</i>                          |
| HTR 2012 conference                   | The IAEA Coordinated Research Program on HTGR Reactor Physics, Thermal-hydraulics and Depletion Uncertainty Analysis                                 | Reitsma, F. et al.                    | <i>Proceedings of HTR 2012, Tokyo, Japan, 2012.</i>                           |

The propagation of cross-section and thermal fluid uncertainties to the coupled steady-state and transient models are the primary contributions of this research. The following models were used as building blocks in this process:

- The Phase I KENO-VI and Serpent2 models (Section 5.2) were developed by Bostelmann (Bostelmann et al., 2016) and were used in this work for comparison with NEWT models. Only the data from the NEWT models were subsequently used in Phases II-IV.
- The PHISICS/RELAP5-3D model was originally jointly developed by Epiney and Strydom for the OECD/NEA MHTGR-350 benchmark (Strydom et al., 2015). It was modified for the HTGR UAM purpose by Strydom and used as the nominal basis for all calculations performed in Chapters 4-6.
- The NEWT few-group cross-section libraries generated in Phase I were utilized in the same PHISICS model using a Python script developed by Rouxelin as part of his RAVEN/PHISICS interface (Rouxelin, et al., 2018). Rouxelin used these models for the Exercise II-2 isothermal core models to assess the impact of material number density uncertainties and to perform the depletion U/SA for Exercise II-1; none of these aspects were used in this work. Rouxelin did not include the cross-section uncertainty assessment of Phase II-IV in his work scope; this aspect is one of the main contributions of the current work. A summary of the models used and the mapping to the dissertation sections is provided in Table C-2.

Table C-2. Summary of IAEA CRP on HTGR UAM contributions and mapping to dissertation.

| Section                              | HTGR UAM Phase/Exercise and Model                                                               | Code                                 | Primary model developer                                  | Secondary model developer             |
|--------------------------------------|-------------------------------------------------------------------------------------------------|--------------------------------------|----------------------------------------------------------|---------------------------------------|
| <i>MHTGR-350 Phase I</i>             |                                                                                                 |                                      |                                                          |                                       |
| 5.2                                  | Ex. I-2a: Fresh fuel block<br>Ex. I-2b: Depletion of fresh fuel block<br>Ex. I-2c: Supercell    | KENO-VI CE<br>KENO-VI MG<br>Serpent2 | Bostelmann                                               | Strydom                               |
| 5.2                                  | Ex. I-2a, I-2b: Fresh & depleted fuel blocks                                                    | NEWT                                 | Rouxelin                                                 | Strydom                               |
| 5.2                                  | Ex. I-2c: Supercell                                                                             | NEWT                                 | Rouxelin                                                 | Strydom                               |
| <i>MHTGR-350 Phase II</i>            |                                                                                                 |                                      |                                                          |                                       |
| 6.2                                  | Ex. II-2a, II-2b: Stand-alone core neutronics<br>(cross-section perturbations)                  | PHISICS/RELAP5-3D (isothermal)       | Epiney (RELAP5-3D nominal)<br>Rouxelin (PHISICS nominal) | Strydom (perturbations)               |
| 7.4                                  | Ex. II-4: Stand-alone core thermal fluids<br>(thermal fluid perturbations)                      | RELAP5-3D                            | Strydom                                                  | -                                     |
| <i>MHTGR-350 Phases III &amp; IV</i> |                                                                                                 |                                      |                                                          |                                       |
| 8.1                                  | Ex. III-1: Coupled core neutronics/thermal fluids (cross-section perturbations)                 | PHISICS/RELAP5-3D                    | Strydom                                                  | -                                     |
| 8.1                                  | Ex. III-1: Coupled core neutronics/thermal fluids (cross-section & thermal fluid perturbations) | PHISICS/RELAP5-3D                    | Strydom                                                  | -                                     |
| 7.5                                  | Ex. IV-1: DLOFC                                                                                 | RELAP5-3D                            | Strydom                                                  | -                                     |
| 8.2                                  | Ex. IV-2: CRW                                                                                   | PHISICS/RELAP5-3D                    | Strydom                                                  | -                                     |
| <i>VHTRC</i>                         |                                                                                                 |                                      |                                                          |                                       |
| 4.3                                  | VHTRC                                                                                           | Serpent2, KENO-VI, TSUNAMI           | Bostelmann                                               | Strydom                               |
| 4.3                                  | VHTRC                                                                                           | NEWT, PHISICS                        | Rouxelin (material uncertainties)                        | Strydom (cross-section uncertainties) |
| All                                  | MHTGR-350, VHTRC                                                                                | RAVEN                                | Strydom                                                  | -                                     |

## **Appendix D: Supplemental Results**

This appendix contains additional data for the IAEA CRP on HTGR UAM exercises that could be of archival value to other participants in the benchmark. The figure and tables are referenced in the main body of this dissertation and are presented without further discussion.

## D-1. Phase III-1

Table D-1. Comparison of 2- and 8-group fuel-temperature mean (K) and standard deviation (%) values for Exercise III-1a (cross-section perturbations only).

| Axial level | 8g_XS fuel temp. $\mu$ (K) |     |     | 2g_XS fuel temp. $\mu$ (K) |      |     | 8g_XS fuel temp. $\sigma$ (%) |      |      | 2g_XS fuel temp. $\sigma$ (%) |      |      |
|-------------|----------------------------|-----|-----|----------------------------|------|-----|-------------------------------|------|------|-------------------------------|------|------|
|             | FR1                        | FR2 | FR3 | FR1                        | FR2  | FR3 | FR1                           | FR2  | FR3  | FR1                           | FR2  | FR3  |
| 1           | 872                        | 749 | 742 | 849                        | 751  | 729 | 0.24                          | 0.22 | 0.21 | 0.25                          | 0.22 | 0.19 |
| 2           | 975                        | 810 | 812 | 951                        | 819  | 798 | 0.20                          | 0.23 | 0.18 | 0.24                          | 0.24 | 0.18 |
| 3           | 1045                       | 854 | 861 | 1020                       | 868  | 847 | 0.16                          | 0.21 | 0.15 | 0.20                          | 0.22 | 0.15 |
| 4           | 1089                       | 882 | 892 | 1064                       | 900  | 881 | 0.12                          | 0.19 | 0.11 | 0.16                          | 0.19 | 0.11 |
| 5           | 1122                       | 906 | 920 | 1098                       | 927  | 910 | 0.08                          | 0.16 | 0.07 | 0.12                          | 0.15 | 0.07 |
| 6           | 1152                       | 931 | 952 | 1128                       | 953  | 943 | 0.05                          | 0.14 | 0.03 | 0.09                          | 0.12 | 0.03 |
| 7           | 1176                       | 951 | 976 | 1151                       | 975  | 968 | 0.05                          | 0.11 | 0.04 | 0.07                          | 0.09 | 0.05 |
| 8           | 1191                       | 964 | 990 | 1166                       | 989  | 983 | 0.06                          | 0.09 | 0.07 | 0.07                          | 0.07 | 0.07 |
| 9           | 1196                       | 971 | 997 | 1173                       | 996  | 991 | 0.07                          | 0.07 | 0.09 | 0.07                          | 0.05 | 0.10 |
| 10          | 1198                       | 976 | 999 | 1174                       | 1001 | 993 | 0.09                          | 0.05 | 0.12 | 0.07                          | 0.04 | 0.13 |

Table D-2. Comparison of 2- and 8-group power mean (MW) and standard deviation (%) values for Exercise III-1a (cross-section perturbations only).

| Axial level | 8g_XS power $\mu$ (MW) |       |       | 2g_XS power $\mu$ (MW) |       |       | 8g_XS power $\sigma$ (%) |      |      | 2g_XS power $\sigma$ (%) |      |      |
|-------------|------------------------|-------|-------|------------------------|-------|-------|--------------------------|------|------|--------------------------|------|------|
|             | FR1                    | FR2   | FR3   | FR1                    | FR2   | FR3   | FR1                      | FR2  | FR3  | FR1                      | FR2  | FR3  |
| 1           | 17.82                  | 17.13 | 18.23 | 16.64                  | 17.20 | 17.03 | 0.65                     | 0.76 | 0.76 | 0.97                     | 1.03 | 1.02 |
| 2           | 18.09                  | 17.01 | 19.04 | 17.22                  | 17.62 | 18.12 | 0.45                     | 0.67 | 0.51 | 0.77                     | 0.87 | 0.77 |
| 3           | 16.61                  | 15.64 | 17.62 | 15.97                  | 16.42 | 17.04 | 0.31                     | 0.56 | 0.33 | 0.54                     | 0.64 | 0.49 |
| 4           | 14.17                  | 13.36 | 15.12 | 13.76                  | 14.23 | 14.88 | 0.25                     | 0.45 | 0.17 | 0.31                     | 0.40 | 0.18 |
| 5           | 11.92                  | 11.32 | 12.93 | 11.67                  | 12.19 | 12.92 | 0.31                     | 0.40 | 0.21 | 0.29                     | 0.33 | 0.27 |
| 6           | 10.20                  | 9.97  | 11.99 | 10.01                  | 10.80 | 12.06 | 0.46                     | 0.42 | 0.42 | 0.54                     | 0.54 | 0.65 |
| 7           | 8.68                   | 8.61  | 10.61 | 8.50                   | 9.34  | 10.72 | 0.62                     | 0.51 | 0.64 | 0.80                     | 0.81 | 0.98 |
| 8           | 7.12                   | 7.07  | 8.74  | 6.97                   | 7.71  | 8.88  | 0.78                     | 0.65 | 0.85 | 1.05                     | 1.08 | 1.28 |
| 9           | 5.50                   | 5.45  | 6.73  | 5.42                   | 5.98  | 6.89  | 0.99                     | 0.83 | 1.09 | 1.31                     | 1.34 | 1.58 |
| 10          | 4.14                   | 4.22  | 4.97  | 4.10                   | 4.59  | 5.12  | 1.41                     | 1.27 | 1.53 | 1.69                     | 1.71 | 1.97 |

Table D-3. Comparison of 2- and 8-group fuel-temperature mean (K) and standard deviation (%) values for Exercise III-1c (cross-section and thermal fluid perturbations).

| Axial level | 8g_XS_TF fuel temp. $\mu$ (K) |     |     | 2g_XS_TF fuel temp. $\mu$ (K) |      |     | 8g_XS_TF fuel temp. $\sigma$ (%) |      |      | 2g_XS_TF fuel temp. $\sigma$ (%) |      |      |
|-------------|-------------------------------|-----|-----|-------------------------------|------|-----|----------------------------------|------|------|----------------------------------|------|------|
|             | FR1                           | FR2 | FR3 | FR1                           | FR2  | FR3 | FR1                              | FR2  | FR3  | FR1                              | FR2  | FR3  |
| 1           | 871                           | 748 | 741 | 848                           | 751  | 728 | 1.15                             | 1.02 | 0.99 | 1.37                             | 1.21 | 1.12 |
| 2           | 974                           | 809 | 812 | 950                           | 818  | 798 | 1.19                             | 1.04 | 1.00 | 1.42                             | 1.26 | 1.18 |
| 3           | 1044                          | 853 | 860 | 1018                          | 867  | 846 | 1.19                             | 1.05 | 1.01 | 1.38                             | 1.26 | 1.18 |
| 4           | 1088                          | 882 | 892 | 1063                          | 899  | 880 | 1.20                             | 1.07 | 1.02 | 1.33                             | 1.22 | 1.15 |
| 5           | 1121                          | 906 | 919 | 1097                          | 926  | 909 | 1.24                             | 1.10 | 1.06 | 1.29                             | 1.20 | 1.13 |
| 6           | 1151                          | 930 | 951 | 1128                          | 953  | 942 | 1.32                             | 1.17 | 1.12 | 1.29                             | 1.21 | 1.14 |
| 7           | 1176                          | 950 | 975 | 1152                          | 975  | 967 | 1.42                             | 1.25 | 1.18 | 1.33                             | 1.25 | 1.17 |
| 8           | 1191                          | 964 | 990 | 1167                          | 989  | 983 | 1.49                             | 1.31 | 1.23 | 1.39                             | 1.30 | 1.20 |
| 9           | 1196                          | 971 | 997 | 1174                          | 996  | 990 | 1.52                             | 1.35 | 1.26 | 1.43                             | 1.33 | 1.23 |
| 10          | 1198                          | 976 | 999 | 1175                          | 1001 | 993 | 1.54                             | 1.37 | 1.27 | 1.45                             | 1.35 | 1.24 |

Table D-4. Comparison of 2- and 8-group power mean (MW) and standard deviation (%) values for Exercise III-1c (cross-section and thermal fluid perturbations).

| Axial level | 8g_XS_TF power $\mu$ (MW) |       |       | 2g_XS_TF power $\mu$ (MW) |       |       | 8g_XS_TF power $\sigma$ (%) |      |      | 2g_XS_TF power $\sigma$ (%) |      |      |
|-------------|---------------------------|-------|-------|---------------------------|-------|-------|-----------------------------|------|------|-----------------------------|------|------|
|             | FR1                       | FR2   | FR3   | FR1                       | FR2   | FR3   | FR1                         | FR2  | FR3  | FR1                         | FR2  | FR3  |
| 1           | 17.76                     | 17.07 | 18.18 | 16.57                     | 17.14 | 16.97 | 2.64                        | 2.83 | 2.88 | 3.41                        | 3.56 | 3.59 |
| 2           | 18.04                     | 16.96 | 18.99 | 17.15                     | 17.56 | 18.04 | 2.35                        | 2.49 | 2.49 | 3.01                        | 3.16 | 3.19 |
| 3           | 16.57                     | 15.61 | 17.58 | 15.91                     | 16.37 | 16.98 | 2.12                        | 2.23 | 2.23 | 2.56                        | 2.71 | 2.74 |
| 4           | 14.15                     | 13.34 | 15.09 | 13.73                     | 14.19 | 14.84 | 1.99                        | 2.07 | 2.07 | 2.13                        | 2.28 | 2.32 |
| 5           | 11.92                     | 11.32 | 12.92 | 11.66                     | 12.18 | 12.90 | 2.05                        | 2.09 | 2.09 | 1.84                        | 1.97 | 2.04 |
| 6           | 10.21                     | 9.97  | 12.00 | 10.02                     | 10.81 | 12.06 | 2.43                        | 2.33 | 2.32 | 1.85                        | 1.94 | 2.04 |
| 7           | 8.69                      | 8.62  | 10.62 | 8.54                      | 9.37  | 10.75 | 3.02                        | 2.70 | 2.65 | 2.24                        | 2.19 | 2.29 |
| 8           | 7.13                      | 7.08  | 8.75  | 7.02                      | 7.74  | 8.91  | 3.53                        | 3.09 | 3.02 | 2.80                        | 2.58 | 2.66 |
| 9           | 5.51                      | 5.46  | 6.74  | 5.46                      | 6.01  | 6.92  | 3.89                        | 3.41 | 3.35 | 3.26                        | 2.96 | 3.05 |
| 10          | 4.15                      | 4.23  | 4.98  | 4.12                      | 4.62  | 5.14  | 4.23                        | 3.76 | 3.73 | 3.65                        | 3.34 | 3.46 |

Table D-5. NSC and Pearson Correlation Coefficients for three FOMs and five core models.

| Perturbed input parameter                                                   | NSC: Maximum fuel temperature <sup>66</sup> |       |       |          |          | PCC: Maximum fuel temperature |       |       |          |          |
|-----------------------------------------------------------------------------|---------------------------------------------|-------|-------|----------|----------|-------------------------------|-------|-------|----------|----------|
|                                                                             | 2g_TF                                       | 2g_XS | 8g_XS | 2g_XS_TF | 8g_XS_TF | 2g_TF                         | 2g_XS | 8g_XS | 2g_XS_TF | 8g_XS_TF |
| Mass flow rate                                                              | -0.48                                       | -     | -     | -0.48    | -0.50    | -0.32                         | -     | -     | -0.32    | -0.32    |
| Inlet temperature                                                           | 0.41                                        | -     | -     | 0.42     | 0.42     | 0.27                          | -     | -     | 0.28     | 0.26     |
| Total power                                                                 | 0.53                                        | -     | -     | 0.52     | 0.53     | 0.87                          | -     | -     | 0.87     | 0.85     |
| <sup>235</sup> U( $\overline{\nu}$ ) / <sup>235</sup> U( $\overline{\nu}$ ) | -                                           | 0.16  | 0.01  | 0.58     | 0.48     | -                             | 0.08  | -0.07 | 0.07     | 0.06     |
| <sup>239</sup> Pu(n, $\gamma$ ) / <sup>239</sup> Pu(n, $\gamma$ )           | -                                           | 0.02  | 0.01  | 0.06     | 0.06     | -                             | 0.07  | 0.07  | 0.07     | 0.07     |
| <sup>12</sup> C(n,n`)/ <sup>12</sup> C(n,n`)                                | -                                           | 0.01  | 0.01  | 0.07     | 0.11     | -                             | -0.06 | 0.06  | 0.07     | 0.06     |
| NSC: Maximum local power <sup>67</sup>                                      |                                             |       |       |          |          | PCC: Maximum local power      |       |       |          |          |
| Mass flow rate                                                              | 0.15                                        | -     | -     | 0.01     | -0.31    | 0.04                          | -     | -     | 0.01     | -0.07    |
| Inlet temperature                                                           | 0.67                                        | -     | -     | 0.69     | 1.05     | 0.19                          | -     | -     | 0.18     | 0.24     |
| Total power                                                                 | 1.18                                        | -     | -     | 1.17     | 1.50     | 0.84                          | -     | -     | 0.78     | 0.87     |
| <sup>235</sup> U( $\overline{\nu}$ ) / <sup>235</sup> U( $\overline{\nu}$ ) | -                                           | 0.67  | -0.58 | 1.29     | 1.34     | -                             | 0.06  | -0.05 | 0.07     | 0.06     |
| <sup>239</sup> Pu(n, $\gamma$ ) / <sup>239</sup> Pu(n, $\gamma$ )           | -                                           | -0.09 | -0.23 | -0.18    | -0.21    | -                             | -0.06 | -0.26 | -0.31    | 0.93     |
| <sup>12</sup> C(n,n`)/ <sup>12</sup> C(n,n`)                                | -                                           | 0.20  | -0.20 | -0.19    | 0.18     | -                             | 0.06  | -0.09 | -0.30    | -0.08    |
| NSC: Eigenvalue                                                             |                                             |       |       |          |          | PCC: Eigenvalue               |       |       |          |          |
| Mass flow rate                                                              | 0.05                                        | -     | -     | 0.01     | 0.01     | 0.30                          | -     | -     | 0.03     | 0.01     |
| Inlet temperature                                                           | -0.06                                       | -     | -     | -0.06    | -0.06    | -0.38                         | -     | -     | -0.12    | -0.11    |
| Total power                                                                 | -0.05                                       | -     | -     | -0.05    | -0.04    | -0.83                         | -     | -     | -0.26    | -0.22    |
| <sup>235</sup> U( $\overline{\nu}$ ) / <sup>235</sup> U( $\overline{\nu}$ ) | -                                           | 0.65  | 0.65  | 0.64     | 0.63     | -                             | 0.58  | 0.58  | 0.54     | 0.54     |
| <sup>239</sup> Pu(n, $\gamma$ ) / <sup>239</sup> Pu(n, $\gamma$ )           | -                                           | -0.10 | -0.10 | -0.11    | -0.11    | -                             | -0.31 | -0.30 | -0.31    | -0.32    |
| <sup>238</sup> U(n, $\gamma$ ) / <sup>238</sup> U(n, $\gamma$ )             | -                                           | -0.06 | -0.06 | -0.06    | -0.06    | -                             | -0.30 | -0.28 | -0.30    | -0.29    |

<sup>66</sup> The maximum fuel temperature occurs in axial level 10 of Fuel Ring 1<sup>67</sup> The maximum power production occurs in axial level 2 in Fuel Ring 3

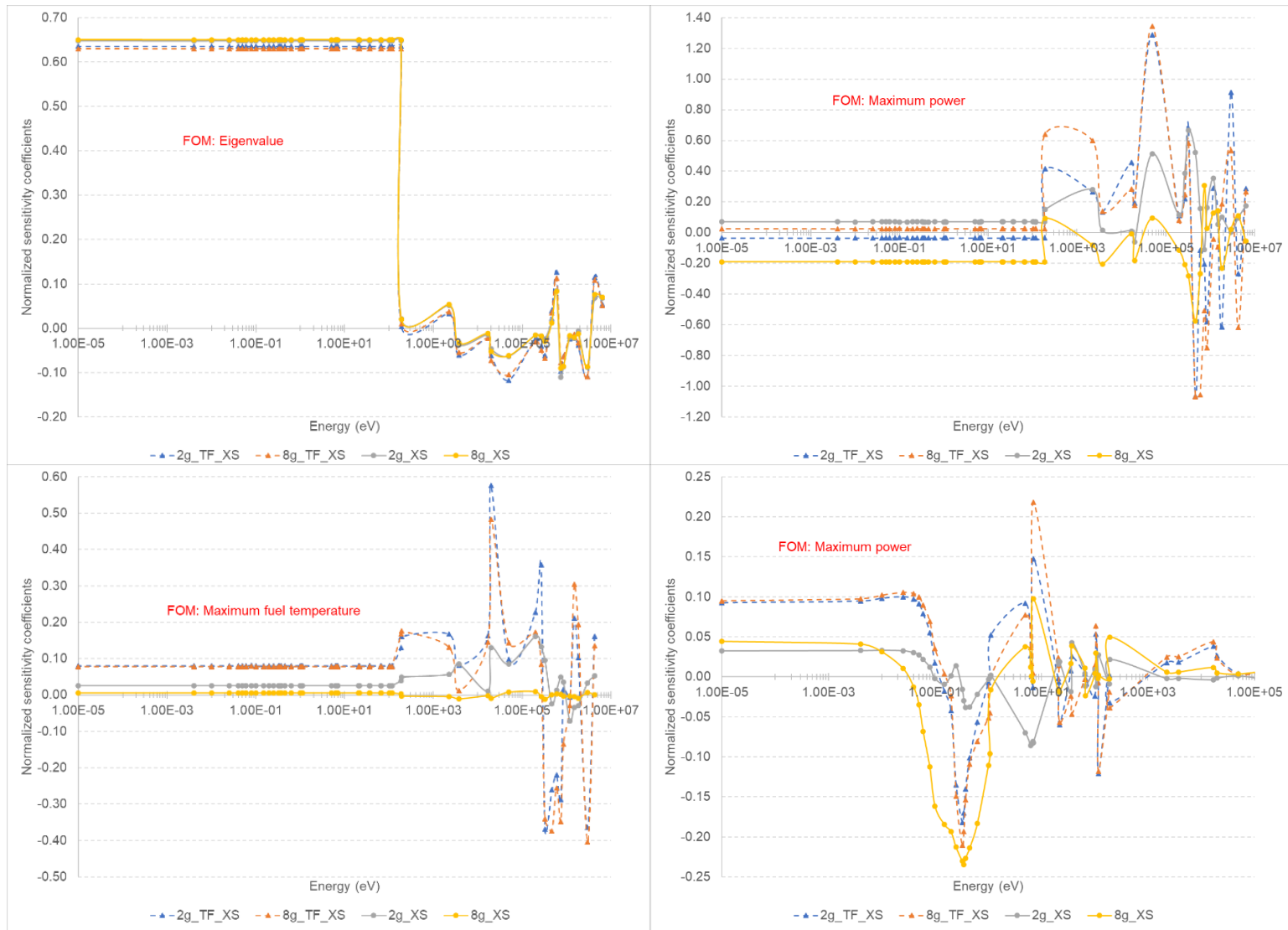


Figure D-1.  $^{235}\text{U}(\bar{\nu}) / ^{235}\text{U}(\bar{\nu})$  (top left and right, bottom left) and  $^{239}\text{Pu}(n,\gamma) / ^{239}\text{Pu}(n,\gamma)$  (bottom right) normalised sensitivity coefficients for three FOMs as a function of energy (eV).

## D-2. Phase IV-2

Table D-6. Exercise IV-2 mean fuel temperature (K) and core power (MW) [top] and standard deviations (%) [bottom].

| Axial level | 8g_XS                                   |      |      | 8g_XS_TF |      |      | 2g_XS_TF |      |      | 8g_XS                             |      |      | 8g_XS_TF |      |      | 2g_XS_TF |      |      |
|-------------|-----------------------------------------|------|------|----------|------|------|----------|------|------|-----------------------------------|------|------|----------|------|------|----------|------|------|
|             | Mean fuel temperature (K) @ 370 s       |      |      |          |      |      |          |      |      | Mean core power (MW) @ 300.5 s    |      |      |          |      |      |          |      |      |
| 1           | 995                                     | 842  | 847  | 996      | 843  | 848  | 970      | 849  | 830  | 40.9                              | 41.6 | 47.9 | 41.8     | 42.5 | 48.9 | 41.9     | 45.8 | 49.2 |
| 2           | 1106                                    | 907  | 927  | 1107     | 908  | 928  | 1079     | 923  | 910  | 41.0                              | 40.6 | 49.2 | 41.9     | 41.5 | 50.3 | 42.1     | 45.5 | 50.9 |
| 3           | 1173                                    | 951  | 975  | 1174     | 951  | 975  | 1143     | 970  | 958  | 37.8                              | 37.5 | 45.7 | 38.7     | 38.3 | 46.7 | 38.6     | 42.0 | 47.4 |
| 4           | 1208                                    | 973  | 998  | 1208     | 973  | 998  | 1177     | 994  | 983  | 32.6                              | 32.2 | 39.4 | 33.3     | 33.0 | 40.3 | 33.2     | 36.3 | 41.2 |
| 5           | 1228                                    | 987  | 1013 | 1228     | 987  | 1012 | 1198     | 1010 | 1000 | 27.1                              | 26.8 | 32.8 | 27.7     | 27.4 | 33.5 | 27.6     | 30.2 | 34.5 |
| 6           | 1241                                    | 998  | 1027 | 1241     | 998  | 1026 | 1213     | 1024 | 1016 | 22.0                              | 21.8 | 26.9 | 22.5     | 22.3 | 27.4 | 22.6     | 24.7 | 28.5 |
| 7           | 1249                                    | 1005 | 1034 | 1249     | 1005 | 1034 | 1222     | 1033 | 1025 | 17.5                              | 17.3 | 21.4 | 17.9     | 17.6 | 21.8 | 18.1     | 19.8 | 22.9 |
| 8           | 1249                                    | 1007 | 1035 | 1249     | 1007 | 1034 | 1224     | 1036 | 1028 | 13.6                              | 13.3 | 16.5 | 13.8     | 13.6 | 16.8 | 14.1     | 15.4 | 17.8 |
| 9           | 1242                                    | 1005 | 1030 | 1242     | 1005 | 1029 | 1221     | 1035 | 1026 | 10.0                              | 9.8  | 12.2 | 10.2     | 10.0 | 12.4 | 10.5     | 11.5 | 13.3 |
| 10          | 1234                                    | 1004 | 1023 | 1234     | 1003 | 1022 | 1215     | 1034 | 1020 | 7.3                               | 7.4  | 8.8  | 7.5      | 7.6  | 8.9  | 7.8      | 8.6  | 9.7  |
|             | Fuel temperature standard deviation (%) |      |      |          |      |      |          |      |      | Core power standard deviation (%) |      |      |          |      |      |          |      |      |
| 1           | 0.39                                    | 0.32 | 0.40 | 1.34     | 1.19 | 1.21 | 1.38     | 1.26 | 1.23 | 1.88                              | 1.85 | 2.07 | 3.13     | 3.23 | 3.38 | 2.75     | 2.87 | 3.07 |
| 2           | 0.29                                    | 0.27 | 0.33 | 1.37     | 1.20 | 1.23 | 1.39     | 1.28 | 1.26 | 1.67                              | 1.64 | 1.86 | 2.93     | 2.95 | 3.12 | 2.40     | 2.50 | 2.69 |
| 3           | 0.26                                    | 0.25 | 0.30 | 1.41     | 1.25 | 1.27 | 1.40     | 1.29 | 1.27 | 1.69                              | 1.66 | 1.87 | 3.06     | 3.02 | 3.15 | 2.40     | 2.45 | 2.61 |
| 4           | 0.23                                    | 0.22 | 0.27 | 1.47     | 1.29 | 1.30 | 1.42     | 1.31 | 1.29 | 1.77                              | 1.72 | 1.94 | 3.38     | 3.25 | 3.33 | 2.71     | 2.63 | 2.73 |
| 5           | 0.21                                    | 0.20 | 0.24 | 1.53     | 1.35 | 1.35 | 1.45     | 1.35 | 1.31 | 1.85                              | 1.78 | 2.00 | 3.77     | 3.52 | 3.57 | 3.08     | 2.90 | 2.96 |
| 6           | 0.19                                    | 0.17 | 0.21 | 1.60     | 1.41 | 1.39 | 1.51     | 1.39 | 1.35 | 1.91                              | 1.80 | 2.01 | 4.22     | 3.80 | 3.79 | 3.57     | 3.19 | 3.21 |
| 7           | 0.18                                    | 0.14 | 0.20 | 1.65     | 1.45 | 1.43 | 1.56     | 1.43 | 1.38 | 1.96                              | 1.83 | 2.04 | 4.54     | 4.04 | 4.00 | 3.97     | 3.45 | 3.46 |
| 8           | 0.17                                    | 0.12 | 0.19 | 1.67     | 1.48 | 1.45 | 1.59     | 1.46 | 1.40 | 2.04                              | 1.89 | 2.13 | 4.79     | 4.26 | 4.22 | 4.27     | 3.71 | 3.71 |
| 9           | 0.16                                    | 0.10 | 0.18 | 1.66     | 1.49 | 1.45 | 1.60     | 1.47 | 1.41 | 2.17                              | 2.01 | 2.27 | 5.02     | 4.48 | 4.45 | 4.53     | 3.96 | 3.96 |
| 10          | 0.16                                    | 0.08 | 0.19 | 1.65     | 1.49 | 1.45 | 1.59     | 1.48 | 1.41 | 2.52                              | 2.38 | 2.62 | 5.31     | 4.80 | 4.79 | 4.84     | 4.32 | 4.34 |

Table D-7. Exercise IV-2 fuel temperature and core power difference (%) with 8g\_XS\_TF model for mean  $\mu$  [top] and standard deviation  $\sigma$  [bottom].

| Axial level | 8g_XS                                                  |       |       | 2g_XS_TF |       |       | 8g_XS                                            |      |      | 2g_XS_TF |        |       |
|-------------|--------------------------------------------------------|-------|-------|----------|-------|-------|--------------------------------------------------|------|------|----------|--------|-------|
|             | Fuel temperature $\mu$ difference with 8g_XS_TF (%)    |       |       |          |       |       | Core power $\mu$ difference with 8g_XS_TF (%)    |      |      |          |        |       |
| 1           | 0.12                                                   | 0.07  | 0.09  | 2.63     | -0.77 | 2.05  | 2.11                                             | 2.10 | 2.08 | -0.28    | -7.76  | -0.55 |
| 2           | 0.08                                                   | 0.04  | 0.06  | 2.55     | -1.67 | 1.89  | 2.19                                             | 2.19 | 2.19 | -0.34    | -9.71  | -1.18 |
| 3           | 0.05                                                   | 0.02  | 0.02  | 2.61     | -1.96 | 1.72  | 2.27                                             | 2.25 | 2.24 | 0.21     | -9.67  | -1.55 |
| 4           | 0.02                                                   | -0.01 | -0.01 | 2.54     | -2.20 | 1.48  | 2.23                                             | 2.24 | 2.24 | 0.34     | -9.95  | -2.18 |
| 5           | 0.00                                                   | -0.03 | -0.03 | 2.44     | -2.41 | 1.24  | 2.23                                             | 2.19 | 2.20 | 0.15     | -10.48 | -2.99 |
| 6           | -0.01                                                  | -0.03 | -0.03 | 2.30     | -2.60 | 1.02  | 2.12                                             | 2.12 | 2.12 | -0.19    | -11.22 | -3.95 |
| 7           | -0.02                                                  | -0.04 | -0.04 | 2.14     | -2.76 | 0.81  | 2.03                                             | 2.03 | 2.04 | -0.87    | -12.06 | -4.96 |
| 8           | -0.03                                                  | -0.05 | -0.05 | 1.94     | -2.92 | 0.59  | 1.95                                             | 1.96 | 1.97 | -1.83    | -13.16 | -6.09 |
| 9           | -0.03                                                  | -0.05 | -0.05 | 1.72     | -3.05 | 0.38  | 1.90                                             | 1.90 | 1.91 | -3.14    | -14.61 | -7.53 |
| 10          | -0.04                                                  | -0.05 | -0.06 | 1.56     | -3.05 | 0.24  | 1.86                                             | 1.86 | 1.87 | -4.03    | -14.17 | -8.66 |
|             | Fuel temperature $\sigma$ difference with 8g_XS_TF (%) |       |       |          |       |       | Core power $\sigma$ difference with 8g_XS_TF (%) |      |      |          |        |       |
| 1           | 0.95                                                   | 0.87  | 0.82  | -0.04    | -0.07 | -0.02 | 1.25                                             | 1.38 | 1.31 | 0.37     | 0.36   | 0.32  |
| 2           | 1.07                                                   | 0.94  | 0.90  | -0.03    | -0.07 | -0.03 | 1.26                                             | 1.31 | 1.26 | 0.53     | 0.45   | 0.43  |
| 3           | 1.16                                                   | 1.00  | 0.97  | 0.02     | -0.04 | -0.01 | 1.37                                             | 1.36 | 1.28 | 0.66     | 0.57   | 0.54  |
| 4           | 1.23                                                   | 1.07  | 1.03  | 0.05     | -0.02 | 0.01  | 1.61                                             | 1.52 | 1.39 | 0.66     | 0.61   | 0.60  |
| 5           | 1.32                                                   | 1.15  | 1.10  | 0.08     | 0.00  | 0.03  | 1.92                                             | 1.74 | 1.57 | 0.70     | 0.62   | 0.61  |
| 6           | 1.41                                                   | 1.24  | 1.18  | 0.09     | 0.02  | 0.04  | 2.31                                             | 1.99 | 1.78 | 0.65     | 0.61   | 0.58  |
| 7           | 1.47                                                   | 1.31  | 1.23  | 0.09     | 0.02  | 0.05  | 2.58                                             | 2.20 | 1.96 | 0.56     | 0.58   | 0.54  |
| 8           | 1.50                                                   | 1.36  | 1.26  | 0.08     | 0.02  | 0.05  | 2.75                                             | 2.37 | 2.10 | 0.52     | 0.55   | 0.52  |
| 9           | 1.51                                                   | 1.39  | 1.27  | 0.07     | 0.02  | 0.04  | 2.85                                             | 2.46 | 2.18 | 0.49     | 0.52   | 0.49  |
| 10          | 1.49                                                   | 1.41  | 1.26  | 0.06     | 0.01  | 0.04  | 2.78                                             | 2.41 | 2.16 | 0.47     | 0.48   | 0.44  |

Table D-8. Exercise IV-2 Total power and MFT PCC and NSC data for five core models.

| Perturbed input variable                                                | Metric | 2g_TF                                         |       | Rank  | 2g_XS |      | Rank  | 2g_XS_TF |       | Rank  | 8g_XS |      | Rank  | 8g_XS_TF |       | Rank |  |
|-------------------------------------------------------------------------|--------|-----------------------------------------------|-------|-------|-------|------|-------|----------|-------|-------|-------|------|-------|----------|-------|------|--|
|                                                                         |        | Min.                                          | Max.  |       | Min.  | Max. |       | Min.     | Max.  |       | Min.  | Max. |       | Min.     | Max.  |      |  |
|                                                                         |        | Total power at t = 300.5 seconds              |       |       |       |      |       |          |       |       |       |      |       |          |       |      |  |
| Mass flow rate                                                          | PCC    | -0.13                                         | 0.03  | 3     | -     | -    | -     | -0.17    | 0.03  | 2     | -     | -    | -     | -0.18    | 0.10  | 2    |  |
| Inlet gas temperature                                                   |        | -0.03                                         | 0.13  | 2     | -     | -    | -     | -0.02    | 0.14  | 3     | -     | -    | -     | -0.08    | 0.17  | 3    |  |
| Total power                                                             |        | 0.38                                          | 1.00  | 1     | -     | -    | -     | 0.37     | 1.00  | 1     | -     | -    | -     | 0.77     | 1.00  | 1    |  |
| $^{235}\text{U}(\overline{\nu}) / ^{235}\text{U}(\overline{\nu})$       |        | -                                             | -     | -     | -0.14 | 0.16 | 3     | -0.07    | 0.07  | 6     | -0.16 | 0.14 | 3     | -0.08    | 0.07  | 6    |  |
| $^{238}\text{U}(\text{n},\gamma) / ^{238}\text{U}(\text{n},\gamma)$     |        | -                                             | -     | -     | -0.20 | 0.24 | 2     | -0.08    | 0.09  | 5     | -0.18 | 0.18 | 2     | -0.08    | 0.09  | 5    |  |
| $^{239}\text{Pu}(\text{n},\gamma) / ^{239}\text{Pu}(\text{n},\gamma)$   |        | -                                             | -     | -     | -0.27 | 0.32 | 1     | -0.11    | 0.07  | 4     | -0.51 | 0.26 | 1     | -0.12    | 0.10  | 4    |  |
| Mass flow rate                                                          | NSC    | -0.40                                         | 0.09  | 3     | -     | -    | -     | -0.50    | 0.09  | 3     | -     | -    | -     | -0.60    | 0.27  | 3    |  |
| Inlet temperature                                                       |        | -0.12                                         | 0.41  | 2     | -     | -    | -     | -0.06    | 0.43  | 4     | -     | -    | -     | -0.23    | 0.59  | 4    |  |
| Total power                                                             |        | 0.89                                          | 1.08  | 1     | -     | -    | -     | 0.89     | 1.08  | 2     | -     | -    | -     | 0.98     | 1.23  | 2    |  |
| $^{235}\text{U}(\overline{\nu}) / ^{235}\text{U}(\overline{\nu})$       |        | -                                             | -     | -     | -1.05 | 1.11 | 1     | -2.51    | 1.22  | 1     | -0.86 | 0.56 | 1     | -1.30    | 1.24  | 1    |  |
| $^{12}\text{C}(\text{n},\text{n}') / ^{12}\text{C}(\text{n},\text{n}')$ |        | -                                             | -     | -     | -0.09 | 0.31 | 4     | -0.16    | 0.21  | 5     | -0.22 | 0.07 | 2     | -0.02    | 0.31  | 5    |  |
| $^{238}\text{U}(\text{n},\gamma) / ^{238}\text{U}(\text{n},\gamma)$     |        | -                                             | -     | -     | -0.09 | 0.35 | 3     | -0.13    | 0.17  | 7     | -0.05 | 0.06 | 4     | -0.20    | 0.11  | 7    |  |
| $^{239}\text{Pu}(\text{n},\gamma) / ^{239}\text{Pu}(\text{n},\gamma)$   | -      | -                                             | -     | -0.16 | 0.54  | 2    | -0.20 | 0.21     | 6     | -0.20 | 0.12  | 3    | -0.25 | 0.23     | 6     |      |  |
|                                                                         |        | Maximum fuel temperature at t = 370.0 seconds |       |       |       |      |       |          |       |       |       |      |       |          |       |      |  |
| Mass flow rate                                                          | PCC    | -0.32                                         | -0.31 | 2     | -     | -    |       | -0.32    | -0.30 | 2     | -     | -    |       | -0.33    | -0.31 | 2    |  |
| Inlet temperature                                                       |        | 0.26                                          | 0.28  | 3     | -     | -    |       | 0.27     | 0.28  | 3     | -     | -    |       | 0.26     | 0.27  | 3    |  |
| Total power                                                             |        | 0.86                                          | 0.89  | 1     | -     | -    |       | 0.86     | 0.89  | 1     | -     | -    |       | 0.86     | 0.89  | 1    |  |
| $^{235}\text{U}(\overline{\nu}) / ^{235}\text{U}(\overline{\nu})$       |        | -                                             | -     |       | -0.06 | 0.06 | 3     | -0.06    | 0.07  | 4     | -0.08 | 0.05 | 3     | -0.06    | 0.08  | 4    |  |
| $^{238}\text{U}(\text{n},\gamma) / ^{238}\text{U}(\text{n},\gamma)$     |        | -                                             | -     |       | -0.09 | 0.20 | 2     | -0.05    | 0.07  | 6     | -0.11 | 0.10 | 2     | -0.06    | 0.07  | 6    |  |
| $^{239}\text{Pu}(\text{n},\gamma) / ^{239}\text{Pu}(\text{n},\gamma)$   |        | -                                             | -     |       | -0.38 | 0.19 | 1     | -0.06    | 0.07  | 5     | -0.29 | 0.13 | 1     | -0.04    | 0.08  | 5    |  |
| Mass flow rate                                                          | NSC    | -0.53                                         | -0.46 | 2     | -     | -    |       | -0.52    | -0.46 | 3     | -     | -    |       | -0.57    | -0.49 | 3    |  |
| Inlet gas temperature                                                   |        | 0.41                                          | 0.47  | 3     | -     | -    |       | 0.42     | 0.48  | 4     | -     | -    |       | 0.43     | 0.49  | 4    |  |
| Total power                                                             |        | 0.53                                          | 0.58  | 1     | -     | -    |       | 0.53     | 0.58  | 2     | -     | -    |       | 0.56     | 0.61  | 2    |  |
| $^{235}\text{U}(\overline{\nu}) / ^{235}\text{U}(\overline{\nu})$       |        | -                                             | -     |       | -0.09 | 0.08 | 1     | -0.46    | 0.64  | 1     | -0.07 | 0.03 | 1     | -0.53    | 0.65  | 1    |  |
| $^{12}\text{C}(\text{n},\text{n}') / ^{12}\text{C}(\text{n},\text{n}')$ |        | -                                             | -     |       | -0.01 | 0.03 | 3     | -0.02    | 0.11  | 5     | -0.02 | 0.00 | 3     | -0.02    | 0.15  | 5    |  |
| $^{239}\text{Pu}(\text{n},\gamma) / ^{239}\text{Pu}(\text{n},\gamma)$   |        | -                                             | -     |       | -0.02 | 0.03 | 2     | -0.04    | 0.09  | 6     | -0.03 | 0.01 | 2     | -0.04    | 0.11  | 6    |  |