ENGPHYS 4NE3

Advanced Nuclear Engineering

Research Study

Due: Feb 8, 2024

Wonseok Park, 400113079

Muqtadir Hussain, 400250481

Enhancing Power Generation Efficiency in CANDU Reactors: A Study of Fuel Bundle and Reactor Assembly Dynamics Using MCNP Simulation

This report presents an outline of our study on enhancing the efficiency and safety of CANDU (CANada Deuterium Uranium) reactors through advanced simulation techniques using the Monte Carlo N-Particle (MCNP) code. The primary focus is on the reactor's fuel bundle and assembly structures, key components in the reactor's operational efficiency. The study employs MCNP simulations to analyze fission reactions within the reactor, specifically the interactions of neutrons with various nuclear fuels like Uranium-235 (U-235) and Plutonium-239 (Pu-239). By evaluating different fuel candidates and configurations, the research aims to identify optimal setups that maximize power generation while minimizing energy losses. The methodology involves a comprehensive simulation approach, accounting for a large number of sample paths and collisions to ensure statistical accuracy and reliability. Additionally, the study incorporates various uncertainties related to material properties and reactor geometry to provide a realistic and holistic understanding of the reactor's behavior. The expected outcome is to offer insights and recommendations for improving the design and operation of CANDU reactors, contributing to the broader goals of safety, sustainability, and efficiency in nuclear energy production.

Challenges in CANDU Reactor Operation

Despite their advantages, CANDU reactors face challenges in optimizing fuel use, particularly concerning burnup efficiency and fuel management. Ensuring safety in nuclear reactors is also paramount. CANDU reactors, like all nuclear systems, require ongoing attention to safety protocols, especially in the context of radiation management and structural integrity.

Research Gap and Need for Study

There is a continuous need for research to enhance the operational efficiency and safety of CANDU reactors. Advances in simulation technology, particularly Monte Carlo methods, have opened new avenues for such research. The Monte Carlo N-Particle (MCNP) code, known for its accuracy in nuclear simulations, presents an opportunity to study and potentially improve the reactor's fuel bundle and assembly structures, which are crucial for efficient and safe reactor operation.

Purpose of This Study

This report aims to use MCNP simulations to analyze the interactions between neutrons and various nuclear fuels in CANDU reactors. The goal is to evaluate different fuel types and configurations, seeking ways to optimize power generation and minimize energy losses. The findings of this study are anticipated to contribute valuable insights into improving the design and operation of CANDU reactors, aligning with the broader goals of enhancing safety and sustainability in nuclear energy production.

MCNP Simulation:

In our study using the Monte Carlo N-Particle (MCNP) simulation tool, we will be engaging in an in-depth analysis of CANDU reactor physics, with a specific focus on fuel bundle and reactor assembly configurations. The core of our research involves simulating the intricate process of nuclear fission within CANDU reactors. This includes modeling the interactions of neutrons with various fuel types such as Uranium-235 and Plutonium-239, and possibly other heavy nuclear fuels. The goal is to evaluate how these interactions, under different conditions and configurations, impact the reactor's efficiency and safety.

A significant part of our study will be devoted to assessing various fuel candidates, considering how their characteristics influence reactor behavior and overall performance. Through MCNP simulations, we will be able to explore and analyze different configurations of fuel bundles and reactor assemblies. This approach is aimed at identifying the most effective arrangements that could enhance power generation efficiency and minimize energy losses. Additionally, our research will take into account the uncertainties inherent in these simulations, such as variations in material properties and geometrical factors, to ensure a comprehensive and realistic assessment. The outcome of our study is expected to contribute valuable insights into optimizing the design and operation of CANDU reactors, aligning with current efforts to improve the safety and efficiency of nuclear power generation.

Literature Review:

In conducting a comprehensive literature review, several key studies and papers relevant to the field of CANDU reactor efficiency and safety were examined. This review aims to summarize their findings and illustrate how they contribute to the understanding of reactor physics and the challenges faced by CANDU reactors.

Paper [1]:

The first paper, titled "Burnup Calculation of a CANDU6 Reactor Using the Serpent and MCNP6 Codes," presents an in-depth analysis of using the MCNP6 code for fuel burnup calculations in CANDU6 reactors, a critical aspect for assessing reactor efficiency and safety. The study aims to validate the MCNP6 simulations against the Serpent code, emphasizing the importance of precision in these calculations. A notable aspect of the research is its focus on the intricacies of Monte Carlo analyses, particularly highlighting the relationship between the accuracy of results and the number of histories (simulation iterations) used in the simulations. This correlation is crucial since increasing the number of histories can lead to more accurate results, which is fundamental in nuclear reactor simulations where precision is paramount.

The paper also delves into the technical specifics of the simulation process, including the use of thermal scattering data for different reactor components like coolant and moderator. The comparison between MCNP6 and Serpent1.1.19 codes, particularly regarding their treatment of thermal scattering libraries, offers valuable insights into the strengths and limitations of these simulation tools. Overall, this study is significant for our research as it underscores the reliability of MCNP simulations in understanding the complex dynamics of nuclear reactors and contributes to the ongoing efforts to enhance the efficiency and safety of CANDU reactors.

Paper [2]:

The second paper, "MCNP Simulation of In-Core Dose Rates for an Offline CANDU® Reactor," explores the application of the Monte Carlo N-Particle (MCNP) simulation method to predict in-core radiation dose rates in CANDU reactors. This study is particularly relevant in the context of reactor maintenance and safety. One of its key contributions is the development of an MCNP model that is capable of accurately predicting the dose rates various components within the reactor are exposed to, especially during inspection processes. This aspect is crucial for determining the lifetime of these components and ensuring safe operating conditions.

A significant focus of the paper is on enhancing the effectiveness of reactor inspection systems. It discusses a novel approach to inspecting CANDU reactor pressure tubes, including the development of a more advanced robotic inspection system. The MCNP model's ability to predict in-core dose rates informs the design of this inspection system, particularly in terms of shielding requirements for sensitive components. The study demonstrates how MCNP simulations can be employed not just for theoretical analysis but also for practical applications in reactor operations and safety enhancements. This paper's findings underscore the versatility of MCNP simulations in operational safety and engineering solutions, making it a valuable reference for our research on CANDU reactors.

Paper [3]:

The third paper, "Benchmarking of a Generic CANDU Reactor with PARCS, MCNP, and RFSP," addresses the comprehensive benchmarking process of a generic CANDU reactor using a variety of simulation tools, including MCNP (Monte Carlo N-Particle), PARCS, and RFSP. This study is significant for its holistic approach in assessing and comparing the effectiveness of different simulation tools in accurately modeling the physics and operational behavior of CANDU reactors. By employing various tools, the research aims to identify strengths and limitations of each in terms of reactor modeling, thereby contributing to the optimization of reactor design and operations.

A key aspect of this paper is its emphasis on the interplay and validation among multiple simulation methodologies. The research highlights how different tools can complement each other to provide a more nuanced and comprehensive understanding of reactor dynamics. This approach is crucial in the field of nuclear engineering, where the complexity of reactor systems often necessitates a multi-faceted analysis. The paper's findings are particularly relevant for our study, as they demonstrate the value of employing a combination of simulation tools, including MCNP, to gain deeper insights into reactor behavior, fuel efficiency, and safety considerations. This multi-tool benchmarking approach can inform and enhance our MCNP-based study, providing a broader perspective on the potential improvements in CANDU reactors.

Paper [4]:

The fourth paper, "Study of CANDU Thorium-Based Fuel Cycles by Deterministic and Monte Carlo Methods," explores the potential of implementing thorium-based fuel cycles in CANDU reactors. This study is especially relevant in the context of seeking alternative and potentially more efficient fuel sources for nuclear reactors. The research utilizes both deterministic and Monte Carlo methods, including MCNP simulations, to analyze the behavior and efficiency of thorium-based fuel within the CANDU reactor environment. The focus on thorium, an alternative to traditional uranium fuel, indicates a forward-looking approach to nuclear fuel technology, considering factors like sustainability and long-term resource management.

A notable element of this paper is its comparative analysis of thorium-based fuel cycles against conventional uranium cycles in CANDU reactors. This comparison is vital for understanding the potential benefits and challenges of transitioning to alternative fuel sources. The study's findings contribute to a growing body of research that seeks to diversify nuclear fuel options, aiming to enhance reactor efficiency, reduce waste, and address global sustainability concerns. For our research, this paper offers insights into the possibilities and implications of using alternative fuels in CANDU reactors, which could be a significant factor in improving reactor efficiency and sustainability.

Paper [5]:

The fifth paper, “The past, present, and future of nuclear fuel,” considers the most prevalent types of nuclear fuels and their properties with regards to their development process, with snippets of historical context along with it. The article provides some notable insights for the nuclear fuel research towards the near future and concludes with emphasizing the need of modeling and simulation with experiments of the possible fuel candidate, for maximize the energy extraction from them, as well as considering safety and economics.

This article also briefly discusses the efforts made for enhancement of physics-based models with regards to fuel performance versus burnup, and how they can replace the empirical models, enhancing the predictive capabilities of models for fuel performance. Need of quantification of uncertainty related to the development of such models, thus the concepts of Accelerated fuel qualification (AFQ) were introduced, which integrates modeling and simulation with empirical validation to decrease uncertainty and prediction confidence, as well as contributing to economic validity as well.

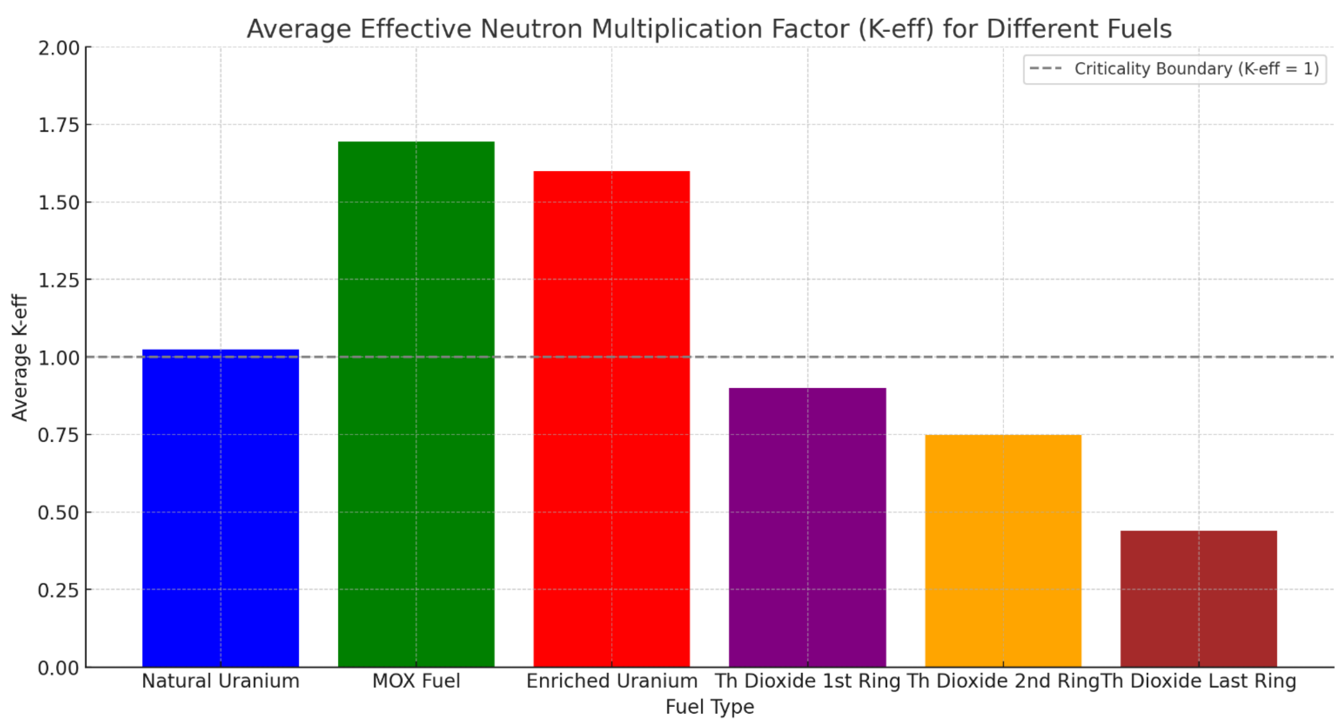
Summary of Reviews/Current Outlook:

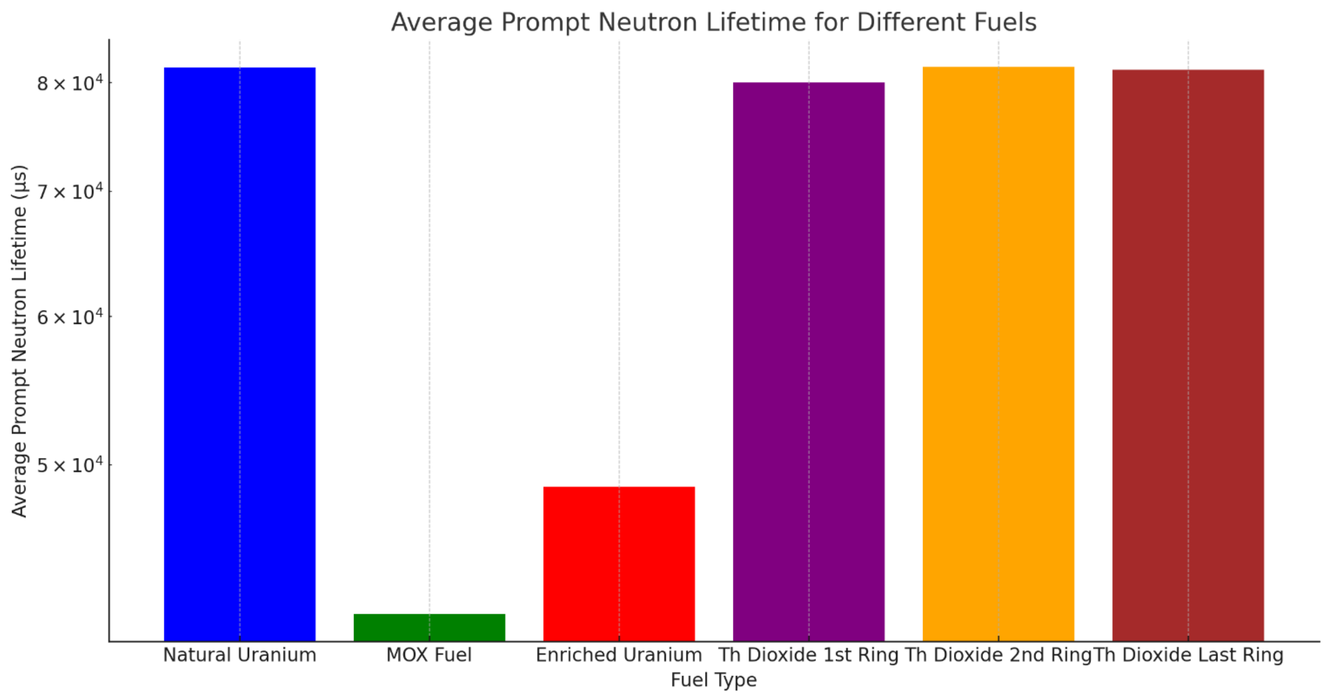
The collective insights from the reviewed papers paint a comprehensive picture of the current challenges and advancements in CANDU reactor technology. These studies highlight the ongoing efforts to optimize reactor efficiency, particularly through precise fuel burnup calculations and the exploration of alternative fuel cycles. The importance of using advanced simulation tools, like MCNP, for accurate modeling and analysis of reactor dynamics is a recurring theme. This approach is critical not only for enhancing fuel efficiency but also for ensuring operational safety, as evidenced by the focus on in-core dose rates and radiation management.

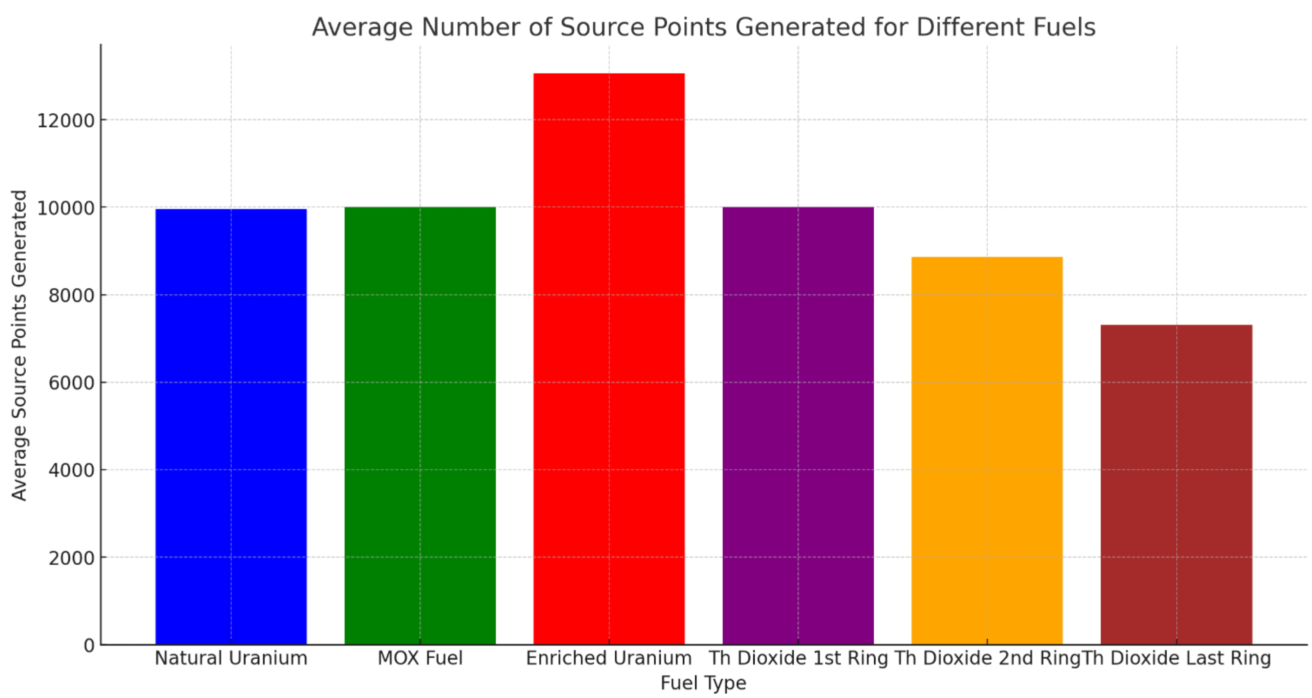
Our research, centered on using MCNP simulations to study the fuel bundle and reactor assemblies in CANDU reactors, directly addresses these challenges. By exploring different fuel types and configurations, our work aims to contribute to the optimization of reactor efficiency and safety. The integration of our study with the broader context of CANDU reactor challenges—such as fuel management, safety considerations, and potential adoption of alternative fuels—positions it as a timely and significant contribution to the field. Our research could provide valuable insights into improving the design and operation of CANDU reactors, aligning with the global objectives of sustainability and efficiency in nuclear energy.

Results:

Fuel Type	Average K-eff	Average Prompt Neutron Lifetime (µs)	Average Source Points Generated
Natural Uranium	1.0240	80,000	9,950
MOX Fuel	1.6935	41,623	10,000.5
Enriched Uranium	1.5986	48,692.5	13,065.5
Thorium Dioxide 1st Ring	0.9000	80,000	10,000
Thorium Dioxide 2nd Ring	0.7480	80,655	8,857
Thorium Dioxide Last Ring	0.4395	81,307.9	7,305.5




Average Prompt Neutron Lifetime for Different Fuels
Average Prompt Neutron Lifetime (μs)
8×10^4
7×10^4
6×10^4
5×10^4
Natural Uranium
MOX Fuel
Enriched Uranium
Th Dioxide 1st Ring
Th Dioxide 2nd Ring
Th Dioxide Last Ring
Fuel Type


Average Number of Source Points Generated for Different Fuels
Average Source Points Generated
12000
10000
8000
6000
4000
2000
0
Natural Uranium
MOX Fuel
Enriched Uranium
Th Dioxide 1st Ring
Th Dioxide 2nd Ring
Th Dioxide Last Ring
Fuel Type

The effective neutron multiplication factor, commonly known as K-eff, is a crucial parameter in nuclear engineering that reflects the state of a nuclear reactor. Here's what the K-eff values indicate for each type of fuel:

1. **Natural Uranium**:
    - The K-eff values around 1.02 suggest that the reactor is slightly supercritical. This means that on average, each fission event leads to slightly more than one subsequent fission event, resulting in a slowly increasing reactor power level. Natural uranium is not as reactive as enriched fuels due to the lower concentration of the fissile isotope U-235.
2. **MOX Fuel (Mixed Oxide Fuel with Plutonium-239 and Uranium-238)**:
    - The higher K-eff values, around 1.68, indicate a significantly supercritical state. MOX fuel contains a mixture of oxides of plutonium (a highly fissile material) and uranium. This high reactivity is due to the presence of Pu-239, which has a higher probability of fission upon neutron absorption than U-238. It means that the neutron population and the power level can increase rapidly unless carefully controlled.
3. **Enriched Uranium**:
    - K-eff values in the range of 1.59 to 1.60 indicate a reactor that is supercritical. Enriched uranium has a higher proportion of the fissile isotope U-235 compared to natural uranium, making it more reactive and capable of sustaining a chain reaction more readily.
4. **Thorium Dioxide in 1st Ring**:
    - A K-eff value around 0.90 suggests a subcritical state. This implies that the chain reaction is not self-sustaining, and the reactor would require an external neutron source or a higher fissile material concentration to reach criticality. Thorium itself is fertile rather than fissile, and thorium reactors typically rely on breeding Th-232 into fissile U-233.
5. **Thorium Dioxide in 2nd Ring**:
    - K-eff values between 0.737 and 0.759 also suggest a subcritical state. Similar to thorium in the first ring, the configuration is such that it does not allow the reactor to reach criticality on its own.
6. **Thorium Dioxide in the Last Ring**:
    - K-eff values ranging from approximately 0.427 to 0.451 are indicative of a strongly subcritical reactor configuration. This is the most subcritical of all configurations discussed and would require significant changes or additional neutron sources to achieve criticality.

In summary, K-eff values above 1.0 denote a supercritical state where the neutron population is increasing over time, values exactly equal to 1.0 denote a critical state where the neutron population is stable, and values below 1.0 denote a subcritical state where the neutron population is decreasing. The K-eff value is crucial for reactor control and safety. A reactor in a supercritical state can lead to an increase in power output, which must be controlled to prevent overheating or an accident. Conversely, a subcritical reactor may require additional measures to sustain a chain reaction for power generation.

The prompt neutron lifetime is a measure of the average time between the emission of a prompt neutron from a fission event and either its absorption in the reactor or its escape from the core. It's a vital parameter in understanding reactor kinetics, and here's what the prompt neutron lifetime values indicate for each fuel type:

1. **Natural Uranium**:
    - With lifetimes around 8×10^4 microseconds, this suggests that neutrons have a relatively long lifespan before they are absorbed or escape. This is typical for reactors with a larger volume and/or a moderator like heavy water that effectively slows down neutrons without absorbing them, as is the case in CANDU reactors. The longer lifetime provides a slower response to changes in reactor control inputs, making the system more stable and easier to control.
2. **MOX Fuel (Mixed Oxide Fuel with Plutonium-239 and Uranium-238)**:
    - The shorter lifetimes, around 4×10^4 microseconds, reflect a more reactive fuel composition due to the inclusion of fissile plutonium. Neutrons in a reactor using MOX fuel are likely to cause further fission or be absorbed more quickly, leading to a faster reactor dynamic. This requires more prompt and precise control mechanisms to maintain the desired reactor state.
3. **Enriched Uranium**:
    - Lifetimes in the order of 4.7×10^4 to 4.9×10^4 microseconds also indicate a relatively short neutron lifespan. Similar to MOX fuel, enriched uranium has a higher proportion of U-235 than natural uranium, increasing the probability of fission and thus reducing the neutron lifetime. This also implies a reactor that responds more quickly to changes in control actions.
4. **Thorium Dioxide in 1st, 2nd, and Last Ring**:
    - For all thorium configurations, the lifetimes are on the higher side, similar to natural uranium, generally above 7.9×10^4 microseconds. Thorium, being a fertile material, doesn't fission as readily as fissile materials. Hence, the neutrons have a longer average lifetime in the reactor. This would generally indicate a more controllable reactor, but given the subcritical state indicated by the K-eff values, it also means that the neutrons are not effectively contributing to a sustained chain reaction.

In practical terms, the prompt neutron lifetime affects how quickly a reactor can change its power level. A shorter lifetime means that the reactor's power can change rapidly, which can be both a challenge in terms of control and an advantage for load-following capabilities. Conversely, a longer lifetime allows for slower, more controllable changes in power but can also imply a less responsive system to sudden demands for power adjustments. It's important to match the design of the reactor control systems to the expected neutron lifetimes to ensure safe and efficient operation.

The number of source points generated in a Monte Carlo N-Particle (MCNP) simulation like those used for evaluating reactor physics refers to the initial locations and energies of neutrons that are sampled to start the chain of reactions in each cycle of the simulation. Here's what these values suggest for each fuel type:

1. **Natural Uranium**:
    - The consistent source points around 9,800 to 10,100 imply that a stable number of neutrons are being sampled for initiating fission events throughout the simulation cycles. It indicates a steady-state operation and a well-characterized neutron distribution for the natural uranium fuel configuration.
2. **MOX Fuel (Mixed Oxide Fuel with Plutonium-239 and Uranium-238)**:
    - The source points, around 9,900 to 10,100, suggest that a similar number of initial neutrons as in the natural uranium case are used to start the fission chain reactions. However, given the higher reactivity of MOX fuel, these neutrons likely lead to more subsequent fission events due to the presence of more fissile plutonium.
3. **Enriched Uranium**:
    - The average of source points, taking into account an outlier, is also in the range of about 13,000 to 10,000. A higher number might indicate a simulation adjusting to a higher neutron flux typical of enriched uranium, which has a greater proportion of fissile U-235. This would be part of the initial condition setting in the simulation to reflect the different reactivity characteristics of the fuel.
4. **Thorium Dioxide in 1st, 2nd, and Last Ring**:
    - The source points for thorium configurations show some variability but are generally around the 10,000 mark, similar to natural uranium. This suggests that despite the subcritical K-eff values, a similar number of initial neutrons are being used to investigate the reactor physics. The variability, especially in the configuration with thorium in the last ring, could be reflective of different simulation conditions or an adjustment to capture the neutronic behavior accurately due to the thorium's properties.

The number of source points generated doesn't directly relate to the fuel's reactivity in a physical reactor but rather reflects the settings of the MCNP simulation to adequately and accurately represent the initiation of neutron events for each cycle. A higher number of source points can improve the statistical accuracy of the simulation results but can also increase computational demands. The goal is to choose a number that balances accuracy with computational efficiency. The consistency in the number of source points across cycles within a simulation is also indicative of the stability and reliability of the simulation conditions.

Conclusion:

The study demonstrates the reactivity and controllability differences between various fuel types in a CANDU reactor. MOX and enriched uranium fuels exhibit higher reactivity, requiring careful control, while natural uranium and thorium dioxide configurations are less reactive, with thorium configurations being subcritical. The results underscore the importance of fuel type in reactor design and operation, where the balance between reactivity (K-eff), neutron economy (prompt neutron lifetime), and simulation accuracy (source points generated) must be carefully managed to achieve desired performance and safety outcomes.

The study indicates that while traditional natural uranium fuel provides stable and efficient operation in CANDU reactors, there are opportunities for enhanced power output and efficiency through the use of MOX or enriched uranium fuels, albeit with necessary considerations for control and safety. Thorium dioxide, despite its lower reactivity, presents interesting potential for future fuel cycle innovations.

References:

[1] Hussein, M. S., Bonin, H. W., & Lewis, B. J. (2014, August 24). *Burnup calculation of a CANDU6 reactor using the serpent and MCNP6 codes*. ResearchGate. https://www.researchgate.net/publication/349683614_Burnup_Calculation_of_a_CANDU6_Reactor_Using_the_Serpent_and_MCNP6_Codes

[2] Gilbert, J. G., Nokleby, S. B., & Waller, E. (2017, May 25). *MCNP Simulation of In-Core Dose Rates for an Offline CANDU® Reactor*. Journal of Nuclear Engineering and Radiation Science. https://doi.org/10.1115/1.4036354

[3] *Benchmarking of a Generic CANDU Reactor with PARCS, MCNP and RFSP (NUREG/IA-0453)*. (n.d.). NRC Web. https://www.nrc.gov/reading-rm/doc-collections/nuregs/agreement/ia0453/index.html

[4] Nuttin, A., Guillemin, P., Courau, T., Marleau, G., Meplan, O., David, S., Michel-Sendis, F., & Wilson, J. N. (2006, July 1). *Study of CANDU thorium-based fuel cycles by deterministic and Monte Carlo methods*. American Nuclear Society, 555 North Kensington Avenue, La Grange Park, IL 60526 (United States). https://www.osti.gov/biblio/22039656

[5] Andersson, D.A., Stanek, C.R., Matthews, C. *et al.* The past, present, and future of nuclear fuel. *MRS Bulletin* **48**, 1154–1162 (2023). https://doi.org/10.1557/s43577-023-00631-3