Assessment of Intra-Pellet Temperature Distribution Effects on Reactivity During RIA Conditions: A Deterministic Analysis Based on the HERA JEEP Benchmark

Alessandro Agostini, Simone Di Pasquale, Marco Cherubini
N.IN.E.
Via della Chiesa XXXII 759, Lucca, Italy;
a.agostini@nineng.com s.dipasquale@nineeng.com m.cherubini@nineng.com

ABSTRACT

Reliable safety assessments of Light Water Reactors (LWRs) under Reactivity Initiated Accident (RIA) conditions require an accurate representation of feedback mechanisms governing core neutronics. Among these, the Doppler effect—strongly dependent on the spatial distribution of fuel temperature—plays a fundamental role in limiting reactivity excursions. While stochastic Monte Carlo codes can naturally account for detailed temperature distributions, conventional deterministic neutronics codes typically approximate the fuel pellet as isothermal, employing a single representative temperature for cross-section generation. This simplification may inadequately describe localized resonance self-shielding phenomena. This work presents an enhanced deterministic neutronics framework modified to explicitly account for the radial temperature distribution within the fuel pellet. The implemented methodology integrates detailed intra-pellet temperature profiles into the generation of homogenized nuclear data, bridging the gap between high-fidelity stochastic modeling and the computational efficiency of deterministic solvers. This enables a more physically consistent treatment of Doppler broadening and neutron interaction probabilities across different fuel regions within a deterministic environment. To assess the impact of this approach, temperature distributions are derived from the High Burnup Experiments for Reactivity Initiated Accident (HERA) Joint Experimental Program (JEEP) Modeling and Simulation (M&S) exercise. Several temperature profiles, each representative of distinct temporal stages of a RIA transient, are considered. Although the present analysis is restricted to steady-state calculations, these snapshots reproduce thermally representative conditions of accident scenarios and allow for a systematic comparison between modeling assumptions. A reactivity-focused comparison is performed between the conventional single-temperature approximation and the distributed-temperature treatment. The analysis quantifies the differences in reactivity insertion associated with the two approaches and evaluates the sensitivity of the results to the severity of the temperature gradient. The findings indicate non-negligible discrepancies in predicted reactivity when spatial temperature effects are explicitly modeled, demonstrating that the isothermal assumption may lead to an underestimation or misrepresentation of Doppler feedback under RIA-relevant conditions. While transient coupling capabilities remain the subject of ongoing development, the present study establishes a clear methodological foundation for high-fidelity accident analysis. The results emphasize the importance of resolving intra-pellet temperature distributions in deterministic reactor simulations and contribute to improving the reliability of safety evaluations within the HERA experimental framework and, more broadly, in LWR accident modelling.

Keywords: *RIA, Doppler feedbacks, LW, HERA*

1 INTRODUCTION

Reactivity Initiated Accidents (RIAs) represent one of the most challenging transient scenarios in Light Water Reactors (LWRs), as they involve rapid positive reactivity insertions that can lead to sharp power excursions within very short time scales. Under such conditions, intrinsic feedback mechanisms play a crucial role in limiting the magnitude of the power pulse and preserving fuel integrity. Among these mechanisms, Doppler broadening of resonance absorption in fertile and fissile isotopes provides the most immediate and robust negative reactivity feedback.

During fast transients such as RIAs, rapid energy deposition combined with the limited thermal conductivity of the fuel can generate significant radial temperature gradients. These gradients directly affect resonance self-shielding behavior so an accurate representation of intra-pellet temperature distributions is therefore essential for a physically consistent evaluation of Doppler feedback during transient conditions.

Despite this physical dependence, most deterministic reactor physics tools treat fuel temperature through simplified assumptions during cross-section generation, typically adopting a single representative temperature for the entire fuel pin. While this effective temperature approach is generally adequate for steady-state applications, it neglects the radial temperature gradients that develop within the fuel pellet, particularly under transient conditions.

Although high-fidelity stochastic transport methods can explicitly account for spatially resolved temperature distributions, their routine application to full-core transient analyses remains computationally demanding. Deterministic nodal solvers therefore remain the primary tools for reactor-scale safety analyses, despite their reliance on the isothermal fuel assumption. The limitations of this simplification have recently received increasing attention within the reactor physics community, as highlighted by the OECD/NEA Task Force on Fuel Temperature Assumptions in Depletion Analyses.

In this context, the present work proposes an enhanced deterministic neutronics methodology that explicitly incorporates radial temperature distributions within the fuel pellet in the generation of homogenized cross sections. The approach is applied to temperature profiles derived from the HERA JEEP Modeling and Simulation exercise, enabling a systematic comparison between conventional isothermal modeling and a distributed-temperature representation under RIA-relevant conditions.

2 HERA BENCHMARK DESCRIPTION

The present study is based on the Modeling and Simulation (M&S) exercise of the High Burnup Experiments for Reactivity Initiated Accident (HERA) Joint Experimental Program [1]. The HERA program, conducted within the NEA FIDES framework, aims to investigate the behavior of Light Water Reactor (LWR) fuel under Reactivity Initiated Accident (RIA) conditions through a combination of experimental activities and coordinated numerical simulations.

The benchmark considers a single fuel rod specimen representative of a typical 17×17 PWR fuel assembly design. The rod consists of fresh UO_2 fuel pellets enclosed in a Zircaloy-4 cladding with a small pellet–cladding gap filled with helium gas. The specimen geometry is specifically designed to reproduce relevant aspects of irradiated fuel behavior, particularly pellet–cladding mechanical interaction (PCMI), by using pre-hydrided cladding and a reduced initial gap.

In this exercise, the transient power history applied to the fuel rod is described by a Gaussian temporal profile, representing the rapid power excursion typical of RIA scenarios. The power pulse is centered at t = 1 s, as shown in Figure 1, corresponding to the time of peak power, while the pulse width is characterized by the Full Width at Half Maximum (FWHM) parameter.

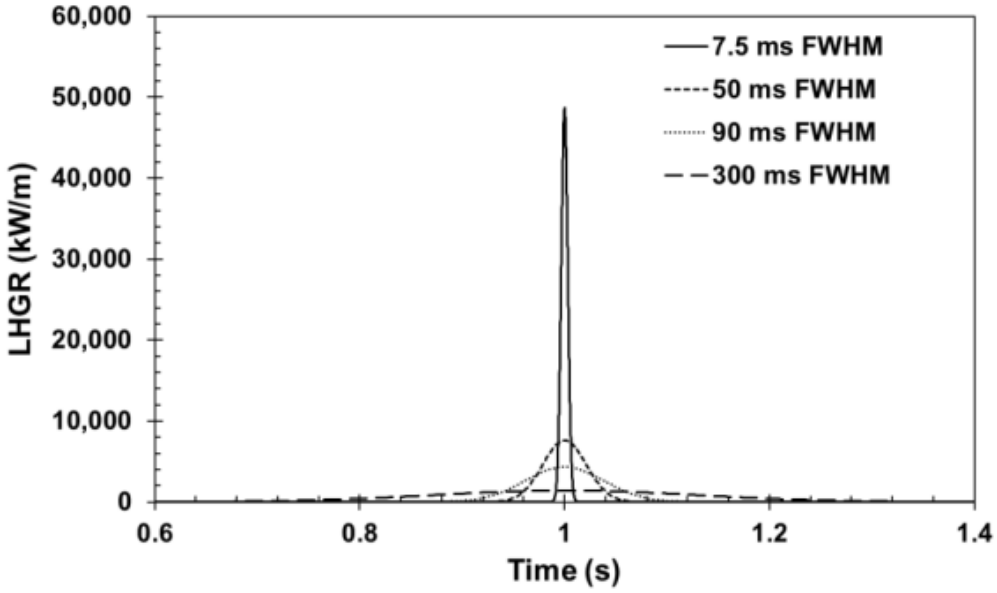

Figure 1: Power Distributions

Several pulse widths and energy depositions are defined in the benchmark in order to explore different accident severities. In particular, the peak radial average fuel enthalpy is varied between 550 J/g, 650 J/g, and 750 J/g, while different pulse widths ranging from a few milliseconds to several hundred milliseconds are considered.

For the purposes of the present work, two representative pulse widths were selected:

- FWHM = 7.5 ms, representing a very sharp and rapid power excursion typical of the most limiting RIA scenarios;
- FWHM = 90 ms, representing an intermediate transient with a slower energy deposition.

To maximize the thermal gradients within the fuel pellet and highlight the impact of temperature distribution on neutronic feedback, the maximum enthalpy case of 750 J/g was selected for both power pulses.

Since the objective of this work is to investigate the impact of intra-pellet temperature distributions on neutronic feedback, specific time instants of the transient were selected in order to extract representative temperature profiles.

For each power pulse, two characteristic times were considered:

- The time corresponding to the peak power, occurring at t = 1.000 s in the benchmark definition.
- The time corresponding to the peak fuel temperature, which occurs slightly after the power peak due to the thermal inertia of the fuel pellet.

The temperature evolution is obtained from fuel performance simulations performed through a coupled RELAP–TRANSURANUS framework, where RELAP provides the thermal-hydraulic boundary conditions while TRANSURANUS computes the detailed thermo-mechanical response of the fuel rod.

Instead of arbitrarily selecting the delay between the power peak and the maximum fuel temperature, a characteristic thermal diffusion time of the fuel pellet was estimated. The radial heat propagation within the pellet can be approximated through the thermal diffusivity of the fuel material, defined as

$$a = \frac{k}{\rho C_p} \quad (1)$$

where k is the thermal conductivity, ρ the fuel density, and Cp the specific heat capacity. The characteristic time required for heat to diffuse across the pellet radius can then be estimated as

$$t_{diff} = \frac{R^2}{a} \quad (2)$$

where R is the fuel pellet radius. This diffusion time provides an estimate of the delay between the instantaneous power deposition and the resulting temperature response within the fuel.

Since the maximum fuel temperature occurs before a complete thermal equilibration of the pellet, the delay between the power peak and the temperature peak was approximated as a fraction of this characteristic diffusion time. Based on this estimation, representative time instants corresponding to the peak fuel temperature were selected shortly after the power peak.

The resulting time points considered in this study are:

- FWHM = 7.5 ms, enthalpy = 750 J/g
  - t = 1.000 s - power peak
  - t = 1.008 s - estimated fuel temperature peak
- FWHM = 90 ms, enthalpy = 750 J/g
  - t = 1.000 s - power peak
  - t = 1.004 s - estimated fuel temperature peak

2.1 Temperature distributions

For each selected transient condition described in the previous section, two different representations of the fuel temperature were considered in the neutronic calculations: a single representative temperature and a radially distributed temperature profile.

The single-temperature approach is based on the concept of an effective or weighted fuel temperature, commonly used in deterministic reactor physics calculations. In this work, the effective temperature is evaluated using the linear Finnemann correlation:

$$T_{eff} = 0.3 \cdot T_{centerline} + 0.7 \cdot T_{surface} \quad (3)$$

where T_c and T_s denote the fuel centerline and surface temperatures, respectively. This formulation has been shown to provide an accurate representation of Doppler feedback under fresh fuel and beginning-of-cycle conditions [2], which are consistent with the benchmark configuration considered in this study.

In contrast, the distributed-temperature approach explicitly accounts for the radial variation of fuel temperature within the pellet. The fuel region is discretized into eight concentric radial zones, each assigned a specific temperature. This choice is based on previous investigations, where it was observed that using between 5 and 10 radial discretization points yields nearly identical neutronic results. Therefore, a discretization into eight regions was adopted as a compromise between numerical accuracy and computational efficiency.

The temperature data obtained from the thermo-mechanical simulations are originally provided at specific radial positions, as shown in table 1.

Table 1: Temperature distributions

FWHM=7.5 ms				**FWHM=90 ms**			
1,000 s		1,008 s		1,000 s		1,004 s	
Radius [mm]	*Temperature [K]*	*Radius [mm]*	*Temperature [K]*	*Radius [mm]*	*Temperature [K]*	*Radius [mm]*	*Temperature [K]*
0.0000	1528.12	0.0000	2485.64	0.0000	1602.71	0.0000	1701.19
0.5253	1527.84	0.5354	2485.6	0.525266	1602.12	0.535418	1700.87
1.0505	1527.85	1.0708	2485.58	1.05053	1601.9	1.07084	1700.64
1.5758	1527.85	1.6063	2485.61	1.5758	1601.88	1.60625	1700.62
2.1011	1527.83	2.1417	2485.48	2.10106	1601.89	2.14167	1700.63
2.6263	1528	2.6771	2486.37	2.62633	1601.87	2.67709	1700.61
3.1516	1526.72	3.2125	2480.59	3.1516	1601.42	3.21249	1700.17
3.6769	1536.33	3.7481	2516.94	3.67689	1611.55	3.74806	1710.94
4.2019	1463.74	4.2825	2278.94	4.20194	1169.264	4.28251	1217.775

It should be noted that the fuel pellet radius slightly varies among the considered cases. While the nominal cold radius is approximately 4.1605 mm, the thermo-mechanical calculations predict an increase in pellet radius due to thermal expansion during the transient.

This increase is a direct consequence of the strong temperature rise in the fuel during the power pulse and is consistent with the thermo-mechanical response predicted by the coupled RELAP–TRANSURANUS simulations. This variation in pellet radius was explicitly accounted for in the neutronic models. However, its impact on the neutronic results is expected to be secondary compared to the effect of temperature on cross sections, since Doppler broadening and resonance self-shielding are primarily driven by temperature rather than by small geometrical changes.

The radial temperature profiles exhibit a characteristic behavior that is consistent across all considered transient conditions. In particular, the temperature remains nearly uniform over a large portion of the pellet radius, followed by a sharper variation in the outer regions. This behavior can be explained by the interplay between volumetric heat generation and radial heat conduction. During the transient, heat is generated relatively uniformly within the fuel volume, while thermal conduction acts to redistribute the energy toward the outer regions. Due to the relatively high thermal conductivity of UO_2 at these temperatures, the inner portion of the pellet tends to remain nearly isothermal. In contrast, steeper temperature gradients develop near the pellet surface, where heat is transferred to the surrounding gap and cladding.

The local maximum observed in the near-peripheral region is associated with the balance between internal heat generation and outward heat removal, while the subsequent temperature drop at the outermost radius reflects the strong cooling effect imposed by the helium gap and cladding interface. This characteristic profile highlights the presence of non-negligible radial temperature gradients, which are expected to significantly influence Doppler broadening and resonance self-shielding effects.

In order to ensure a physically consistent representation within the neutronic model, these temperature values were averaged over the area of each radial region, so that each fuel ring is characterized by a representative mean temperature.

3 NEUTRONIC METHODOLOGY

The neutronic analysis performed in this work relies on a two-step calculation scheme combining Monte Carlo transport simulations for nuclear data generation with deterministic nodal calculations for core neutronic evaluation. In this framework, homogenized few-group cross sections

are first generated using a high-fidelity Monte Carlo model and subsequently employed as input data for the deterministic nodal solver.

3.1 Cross-section generation

Homogenized multi-group cross sections were generated using the Monte Carlo transport code Serpent 2 [3], which is widely used for high-accuracy reactor physics calculations. The simulations were performed under infinite lattice conditions, ensuring that the obtained cross sections represent the local neutronic behavior of the fuel rod independently of global core boundary effects.

The Monte Carlo model represents a single fuel rod surrounded by moderator, consistent with the benchmark configuration described in Section 2. The fuel pellet was radially discretized into several concentric regions in order to represent the intra-pellet temperature distribution, with each region assigned a specific temperature derived from the thermo-mechanical calculations.

In the Serpent framework, spatially varying fuel temperatures can be naturally treated through independent material definitions at different temperatures. Therefore, no modifications to the Monte Carlo code were required to account for the radial temperature distribution within the fuel pellet.

The homogenized cross sections were generated in seven neutron energy groups, providing an adequate resolution of resonance absorption phenomena relevant for Doppler broadening and self-shielding effects.

To reduce the computational cost associated with the cross-section generation process, the homogenization calculations were primarily performed using a two-dimensional model of the fuel rod. Since the neutronic problem considered in this work focuses on radial temperature distributions, the use of a 2D representation provides a physically consistent approximation of the local neutron spectrum within the fuel region.

In order to assess the validity of this approximation, additional three-dimensional Monte Carlo simulations were performed for selected configurations, and the resulting homogenized cross sections were compared with those obtained from the 2D model. The comparison showed very good agreement between the two approaches. For most reaction channels and energy groups, the relative differences remained below 1%, with only limited deviations observed in the highest energy groups where reaction rates are very small. These results confirm that the 2D model provides an accurate and computationally efficient representation for the cross-section generation required in the present study.

3.2 Deterministic nodal calculations

The homogenized cross sections generated with Serpent were subsequently used as input data for the deterministic nodal diffusion solver NEM [4]. This code solves the multi-group neutron diffusion equations using the Nodal Expansion Method, providing an efficient approach for reactor-scale neutronic calculations.

In conventional nodal calculations, the fuel temperature is typically represented through a single effective value associated with the entire fuel region. In order to consistently account for the intra-pellet temperature distributions considered in this work, the NEM code was extended to support multiple temperature points within the fuel pellet.

The implemented modifications allow the solver to handle cross-section data associated with different radial fuel regions, each characterized by its own temperature. To manage the increased dimensionality of the nuclear data, the Nemtab data structure was extended to accommodate a variable number of temperature-dependent parameters. A multidimensional interpolation procedure was also implemented in order to evaluate the appropriate cross sections during the neutronic calculations.

4 RESULTS

As introduced in Section 2.1, the neutronic analysis is based on a comparison between two different fuel temperature representations: a single effective temperature and a radially distributed temperature profile. The impact of these two approaches is evaluated in terms of homogenized cross sections and effective multiplication factor K_{eff}, for the selected transient conditions.

4.1 Cross-section comparison

For the case characterized by FWHM = 7.5 ms, corresponding to the most rapid power excursion, the comparison at t=1.000 s (power peak) shows that the largest discrepancies are observed in the fission cross section, while the total cross section remains almost unaffected, with differences close to zero. This behavior is attributed to internal compensation effects among the various reaction channels.

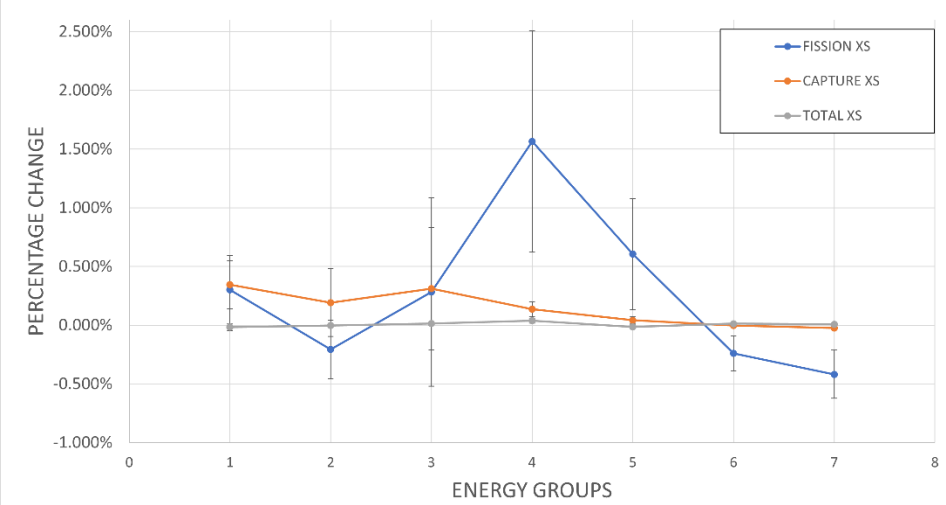

Figure 2: FWHM = 7.5 ms, t=1.000 s

The maximum relative difference in the fission cross section is approximately 1.6% (±1%), with the peak located in energy group 4 (~6.25×10−7 MeV). This energy range corresponds to the epithermal resonance region, where neutron interactions are strongly influenced by the resonance structure of 238U. Since Doppler broadening primarily affects resonance absorption in 238U, the sensitivity to temperature distribution is maximized in this region.

At t=1.008 s, corresponding to the estimated fuel temperature peak, similar trends are observed.

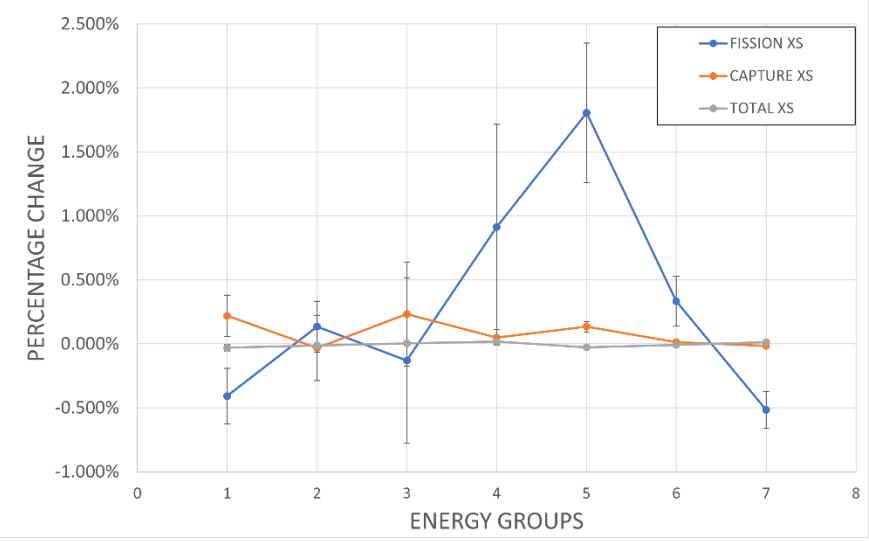

Figure 3: FWHM = 7.5 ms, t=1.008 s

However, the discrepancies slightly increase, with a maximum difference of about 1.8% (±0.5%) in the fission cross section. In this case, the peak shifts toward a lower energy group (~1.4×10−7 MeV). This shift can be explained by the increased fuel temperature, which enhances Doppler broadening and effectively spreads the resonance absorption over a wider energy range, extending its influence toward lower energies.

For the case with FWHM = 90 ms, representing a slower transient, the same general trends are observed for both time instants (t=1.000 s and t=1.004 s), with the largest discrepancies occurring in the fission cross section and negligible differences in the total cross section.

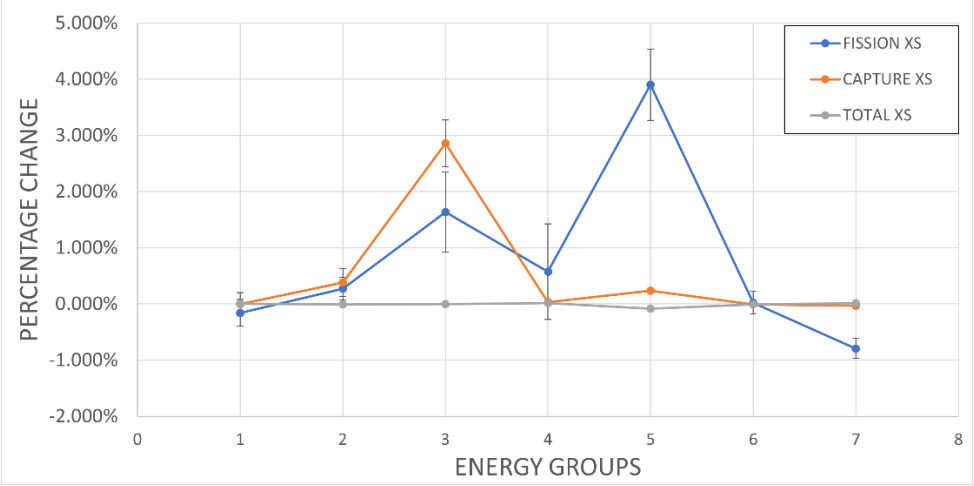

Figure 4: FWHM = 90 ms, t=1.000 s

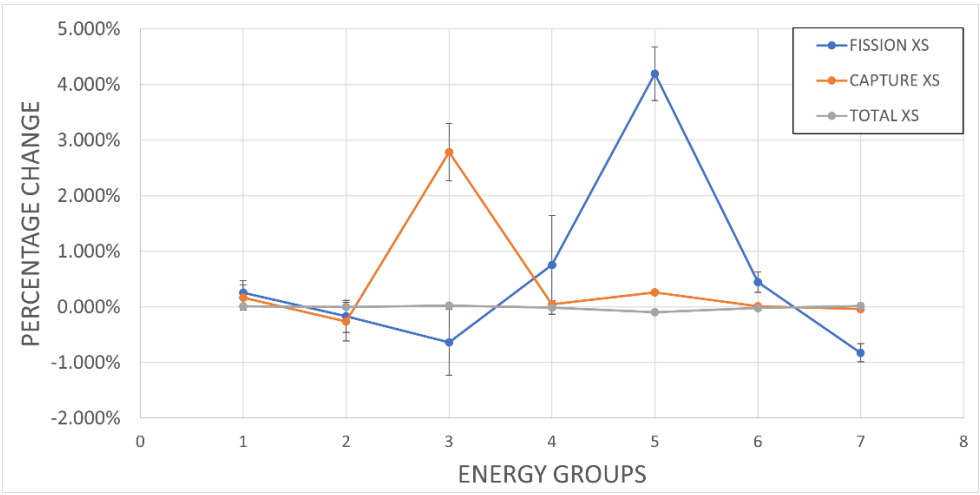

Figure 5: FWHM = 90 ms, t=1.004 s

However, the magnitude of the discrepancies is significantly larger compared to the 7.5 ms case. The maximum relative difference in the fission cross section reaches approximately 4% (±0.6%), again located in the epithermal energy range (group 5). This increase is attributed to the stronger radial temperature gradients that develop during slower transients, leading to a more pronounced difference between the effective temperature and the actual temperature distribution within the fuel.

In addition, a non-negligible discrepancy is observed in the capture cross section, with differences up to 2.8% (±0.5%) in energy group 3 (~4.0×10−6 MeV). This behavior is directly related

to the Doppler effect in 238U, whose resonance absorption dominates in this energy region. Since Doppler broadening is a nonlinear function of temperature, the use of a single effective temperature does not accurately reproduce the spatially varying absorption occurring in the distributed-temperature case. As a result, the averaged cross sections obtained from the two approaches differ significantly, particularly in resonance-dominated energy ranges.

4.2 Reactivity impact

The impact of the different temperature representations on the global neutronic response is evaluated in terms of the effective multiplication factor. Table 2 summarizes the results obtained for all considered cases.

Table 2: Reactivity impact

	Keff		
Case	**1 Temperature**	**8 Temperatures**	**Δ [pcm]**
FWHM = 7.5 – t=1.000s	0.0749147	0.0747170	- 267.6
FWHM = 7.5 – t=1.008s	0.0760052	0.0758275	- 234.35
FWHM = 90 – t=1.000s	0.0751019	0.0747826	- 427.0
FWHM = 90 – t=1.004s	0.0772242	0.0769808	- 316.2

For the 7.5 ms case, a significant discrepancy is observed at the power peak (t=1.000 s), with a difference of approximately -268 pcm, indicating that the single-temperature approach overestimates the reactivity. This result is consistent with an underestimation of Doppler feedback when radial temperature effects are neglected. At the temperature peak (t=1.008 s), a similarly significant discrepancy is observed, with a difference of approximately -234 pcm. This indicates that the impact of the radial temperature distribution remains relevant even at higher fuel temperatures. The slightly reduced magnitude of the discrepancy compared to the power peak can be attributed to partial compensation effects in the neutron balance, although the distributed-temperature representation still leads to a consistently lower reactivity prediction.

For the 90 ms case, the differences are consistently larger, reaching approximately -427 pcm at t=1.000 s and -316 pcm at t=1.004 s. These results clearly indicate that the impact of the temperature distribution on reactivity increases for slower transients. In such conditions, the fuel has more time to develop significant radial temperature gradients, which enhances Doppler broadening effects and amplifies the discrepancy between the single-temperature and distributed-temperature approaches.

From a safety analysis perspective, differences on the order of 300–400 pcm are far from negligible, as they can substantially affect the predicted magnitude of reactivity insertions during RIA scenarios. Such discrepancies are comparable to, or even exceed, typical safety margins and can therefore lead to a misrepresentation of the reactor response under transient conditions. In particular, an overestimation of reactivity may result in an underestimation of the effectiveness of intrinsic feedback mechanisms, such as the Doppler effect, which are crucial for limiting power excursions.

For this reason, achieving a high level of accuracy in the prediction of k_{eff} is of paramount importance in reactor safety analyses. Even relatively small deviations in reactivity can propagate through the calculation chain, ultimately influencing key safety parameters such as peak fuel enthalpy and temperature. The results obtained in this study therefore emphasize that simplifying assumptions in fuel temperature modeling, if not properly addressed, may introduce non-negligible biases in safety evaluations.

A low-power reference condition was also analyzed. Despite the absence of significant power deposition, the fuel temperature profile still exhibits non-negligible radial variations due to thermal boundary conditions. In this case, differences in reactivity of several hundred pcm were observed,

highlighting the strong sensitivity of k_{eff} not only to temperature gradients but also to the definition of the effective fuel temperature.

5 CONCLUSION

This work investigated the impact of radial fuel temperature distributions on neutronic calculations under Reactivity Initiated Accident (RIA) conditions. By comparing a conventional single-temperature approach with a distributed-temperature representation, the study quantified the effects on both homogenized cross sections and global reactivity.

The results show that accounting for intra-pellet temperature gradients leads to non-negligible variations in homogenized cross sections, particularly in resonance energy ranges where Doppler broadening plays a dominant role. The discrepancies are most pronounced in fission and capture cross sections, while total cross sections remain largely unaffected due to compensation effects among reaction channels.

At the core level, these differences translate into significant variations in reactivity, reaching several hundred pcm depending on the transient conditions. In particular, slower transients were found to amplify the impact of temperature distributions, as they allow the development of stronger radial gradients within the fuel pellet. Overall, these results confirm that the impact of radial temperature distributions on cross sections becomes more pronounced as the transient duration increases.

It is worth noting that these discrepancies are observed even in a simplified infinite-lattice configuration based on a single fuel rod, where global core effects such as neutron leakage and spatial heterogeneities are not considered. This suggests that the impact of intra-pellet temperature distributions is intrinsically linked to local neutronic behavior and may remain relevant, or even be amplified, in more realistic full-core simulations.

The present results therefore highlight that the use of a single representative fuel temperature may lead to a systematic overestimation of reactivity, potentially impacting the accuracy of safety evaluations. This finding is particularly relevant for RIA scenarios, where Doppler feedback plays a key role in limiting power excursions.

More generally, this study demonstrates that explicitly resolving intra-pellet temperature distributions improves the physical consistency of deterministic neutronic calculations, bridging the gap with high-fidelity approaches. Future work will focus on extending the methodology to fully coupled transient simulations, in order to assess the dynamic impact of temperature distributions in realistic reactor conditions.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the North Carolina State University (NCSU) for providing the NEM nodal code and for their technical support throughout the development of this work.

REFERENCES

[1] C. Jensen, C. Folsom, D. Kamerman, HERA M&S Exercise Problem Description Report, Idaho National Laboratory, September 2022

[2] H. Finnemann, A. Galati. Neacrp 3-d lwr core transient benchmark. *NEACRP-L-335* (Revision 1), 1992.

[3] J. Leppänen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho. The Serpent Monte Carlo code: Status, development and applications in 2013. *Ann. Nuclear Energy*, 82, 142–150.

[4] Reactor Dynamics and Fuel Management Group (RDFMG). NEM Input User's Manual, vol. 3, 2022. The Pennsylvania State University, Pennsylvania.