Neutronic-Thermal-Hydraulic Coupling of Thermal Expansion Reactivity Feedback in Small Fast Reactors

Authors: Zhang Shenghao, Liu Shichang, Liang Dongsheng, Ma Yugao, Wang Jinyu, Zhang Jingyu, Liu Shichang

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Abstract

Compared with conventional thermal neutron reactors, fast reactors exhibit higher fuel enrichment and a harder neutron spectrum, and the Doppler broadening effect, predominantly arising from U-238, is weaker during reactor operation. Consequently, the impact of core structural deformation on reactivity constitutes a larger fraction of the overall reactivity feedback. Therefore, accurate assessment of the core thermal expansion reactivity feedback effect represents an essential component of fast reactor safety analysis. For fast neutron pulse reactors, criticality calculations for models before and after thermal expansion were performed using the Monte Carlo method, while thermal-mechanical coupling calculations were conducted using the finite element analysis method, thereby enabling nuclear-thermal coupling computational analysis of the thermal expansion reactivity feedback effects for the Godiva-I and Godiva-IV pulse reactors. The calculated fuel reactivity temperature coefficients show good agreement with experimental values, with a maximum relative error of less than 5%, thereby validating the applicability and accuracy of this coupling methodology.

Full Text

Neutronic and Thermal-Mechanical Coupling Study of Thermal Expansion Reactivity Feedback in Small Fast Reactors

ZHANG Shenghao[1], LIU Shichang[1], LIANG Dongsheng[1], MA Yugao[2], WANG Jinyu[2], ZHANG Jingyu[1]

[1] School of Nuclear Science and Engineering, North China Electric Power University, Beijing 100096, China

[2] Nuclear Power Institute of China, Chengdu 610213, China

Abstract

Compared with traditional thermal neutron reactors, fast reactors exhibit higher fuel enrichment and a harder neutron spectrum, resulting in a weaker Doppler broadening effect dominated by U-238 during operation. Consequently, the influence of core structural deformation on reactivity constitutes a larger share of the overall reactivity feedback. Therefore, accurate assessment of core thermal expansion reactivity feedback effects represents a critical component of fast reactor safety analysis. Focusing on fast neutron pulse reactors, this study conducts neutronic-thermal-mechanical coupling calculations and analysis of thermal expansion reactivity feedback effects for the Godiva-I and Godiva-IV pulse reactors using Monte Carlo methods for criticality calculations before and after thermal expansion, and finite element analysis for thermal-mechanical coupling calculations. The results demonstrate that the calculated fuel reactivity temperature coefficients agree well with experimental values, with maximum relative errors within 5%, thereby validating the applicability and accuracy of the coupling methodology.

Keywords: small fast reactors; thermal expansion reactivity feedback effect; neutronic-thermal-mechanical coupling; Godiva-I; Godiva-IV

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Introduction

Small nuclear reactors (micro nuclear reactors) have emerged as critical energy solutions for extreme environment missions such as deep-sea exploration and space exploration, owing to their high energy density, compact structure, and low maintenance requirements. These systems not only provide persistent and stable autonomous power supply for various equipment but also satisfy the flexible deployment demands of high-energy-consumption devices, representing a focal point of international nuclear energy research and development in recent years. Current mainstream micro nuclear reactor technology routes primarily include helium-cooled high-temperature gas-cooled reactors, heat pipe reactors based on heat pipe heat transfer, sodium-cooled/lead-cooled fast reactors with liquid metal coolants, molten salt reactors with inherent safety characteristics, and technologically mature light water reactors, among other types [1].

The aforementioned domestic and international mainstream micro reactor types are predominantly fast neutron reactors. Compared with conventional thermal neutron reactors, fast reactors feature higher fuel enrichment and harder neutron spectra. During normal operation, the Doppler broadening effect dominated by U-238 is relatively weaker in fast reactors than in thermal reactors, making the impact of core structural deformation on reactivity account for a larger proportion of the overall reactivity feedback. Small fast reactors exhibit more complex multi-physics coupling characteristics during operation: beyond the fundamental neutronic-thermal coupling, their compact core structure introduces two novel coupling mechanisms—neutronic-mechanical coupling and thermal-mechanical coupling—forming a strongly coupled system of neutron physics, thermal-hydraulics, and structural mechanics (referred to as neutronic-thermal-mechanical coupling).

Existing research has primarily focused on neutronic-thermal coupling for thermal reactors. Neutronic-thermal coupling methods that neglect geometric deformation feedback (such as density/dimensional changes) lead to reactivity evaluation biases in fast reactors, where issues such as simplified geometric effects and insufficient dynamic coupling exist. Studies specifically addressing neutronic-thermal-mechanical coupling of thermal expansion reactivity feedback effects in fast reactors remain limited. Edward Lum et al. [2] employed Monte Carlo and finite element methods to calculate the reactivity temperature coefficient of the Godiva-IV pulse reactor, performing thermal expansion deformation calculations through ANSYS first, then importing displacement data into MCNP for reactivity temperature coefficient calculations, thereby achieving only stepwise one-way coupling. Manuele Aufiero et al. [3] coupled the Serpent Monte Carlo code with OpenFOAM, utilizing dynamic mesh technology to simulate neutron transport and thermal-mechanical feedback during Godiva-I prompt criticality, though their explicit coupling exhibited insufficient stability under large deformations, requiring manual handling of mesh distortion and resulting in low computational efficiency. Chen Shuo et al. [4] conducted neutronic-thermal-mechanical one-way coupling calculations of fission rates, temperature rise, and stress response for the Godiva-IV pulse reactor based on MCNP and ANSYS; however, they adopted experimentally measured values for the reactivity temperature coefficient and only achieved one-way coupling.

Therefore, to accurately evaluate the reactivity feedback effects of core thermal expansion in small fast reactors, this study constructs a neutronic-thermal-mechanical coupling framework using the Monte Carlo neutron transport code RMC and finite element analysis software ANSYS Mechanical, implementing an automatic coupling iteration process with cell-level temperature/density/displacement mapping and automatic geometry updates. This coupling framework is then applied to perform neutronic-thermal-mechanical coupling calculations for Godiva-I and Godiva-IV pulse reactors, comparing calculated fuel reactivity temperature coefficients with experimental values, analyzing the reactivity feedback effects of thermal expansion, and preliminarily verifying the applicability and accuracy of the coupling method.

1.1 Nuclear Thermal-Mechanical Coupling Framework

The neutronic-thermal-mechanical coupling analysis employs the Monte Carlo code RMC, independently developed by the Department of Engineering Physics at Tsinghua University [5], and the general-purpose finite element analysis software ANSYS Mechanical 17.2. RMC serves as a professional Monte Carlo neutron transport simulation tool capable of accurately modeling neutron physics processes, while ANSYS Mechanical provides mature thermal-mechanical analysis capabilities [6], with their combination enabling multi-physics coupling calculations.

Detailed descriptions of the neutronic-thermal-mechanical coupling calculation method can be found in reference [8]. The coupling calculation process is illustrated in Figure 1 [Figure 1: see original paper]. This study adopts a hybrid coupling mode with RMC as the main program [9], utilizing the Picard iteration method for coupling. The specific coupling process proceeds as follows: RMC first performs neutron transport calculations to obtain the fuel power distribution, which is then processed through the coupling interface and output as a fuel power density information file recognizable by ANSYS. Subsequently, ANSYS is invoked by RMC to read the power density information file and perform thermal-mechanical coupling calculations, yielding temperature, density, and displacement field results for the core, which are written to data files according to the spatial mapping relationship between the finite element mesh model and the CSG model. RMC then checks the signal file and calls the automatic modeling program, which reads the geometric displacement information output by ANSYS and automatically updates the RMC input deck. Finally, RMC reads the geometry-updated input deck and the temperature and density information from the data file output by ANSYS, performs online cross-section broadening and macroscopic cross-section calculations, and re-executes the neutron transport calculation. This process repeats until convergence criteria are met or the maximum number of iterations is reached.

1.2 Spatial Mapping and Data Exchange Method

Both RMC and ANSYS Mechanical achieve cell-level solution accuracy. Figure 2 [Figure 2: see original paper] illustrates the spatial mapping and data exchange method in neutronic-thermal-mechanical coupling using a single fuel pellet as an example. Since RMC constructs computational models using CSG while ANSYS uses finite element meshes, and the number of finite element meshes typically exceeds the number of cells, the spatial mapping relationship in neutronic-thermal-mechanical coupling is a “one-to-many” mapping between RMC cells and ANSYS finite element meshes, with solution accuracy largely dependent on the number of cells in the RMC model.

Regarding data exchange, the fuel power distribution statistically obtained through RMC’ s tally function is processed by the coupling interface into fuel power density and directly assigned to the nodes of the corresponding ANSYS finite element meshes. After ANSYS completes the thermal-mechanical coupling calculation, the volume-averaged temperature and volume of the fuel pellet are calculated through post-processing, where the temperature is used for Doppler cross-section broadening in RMC and the volume is used to solve for the average density based on mass conservation for macroscopic cross-section adjustment in RMC. The average temperature and density calculation formulas are: 1ni-iTTn== where T and represent the average temperature and average density of the cell, respectively; Ti and Vi represent the temperature and density of the i-th mesh node/element mapped to the cell, respectively; n represents the total number of mesh nodes/elements mapped to the cell; and the subscript Initial denotes initial values.

The neutronic-thermal-mechanical coupling feedback mechanism is implemented through dynamic updates of temperature fields, density fields, and geometric parameters in RMC. For thermal feedback, online cross-section broadening technology is employed to handle material Doppler effects: the target motion sampling (TMS) method [10] is used for the resolvable resonance energy region, while probability table interpolation is applied for the unresolvable resonance energy region. For mechanical feedback, geometric deformation feedback is realized through model updates: in this study, for the Godiva-I model, the general spherical equation is updated to describe metal sphere expansion, while for the Godiva-IV model, elliptical equations describe radial geometric expansion of fuel rings and planar equations describe height variations of fuel rings. Density reactivity effects are implemented by modifying macroscopic cross-sections, with the calculation formula as follows:

1.3 Convergence Criteria

Convergence of the neutronic-thermal-mechanical coupling calculations in this study is based on keff convergence, with temperature and displacement changes also serving as criteria for thermal-mechanical coupling convergence. The convergence of relative keff changes between adjacent iteration steps is calculated by the following formula:

where the superscripts n-1, n, and n+1 denote iteration step numbers; the subscript i denotes mesh index; N represents the total number of meshes; and represents the tolerance.

1.4 Reactivity Temperature Coefficient Calculation

The reactivity temperature coefficient is defined as In this coupling method, the first iteration step of RMC employs initial geometry and initial temperature for criticality calculations, while at coupling iteration convergence, RMC uses the temperature and geometry obtained from ANSYS thermal-mechanical coupling calculations for criticality calculations. The reactivity temperature coefficient at neutronic-thermal-mechanical coupling convergence can then be obtained by dividing the keff values from the initial iteration and the converged iteration by the average temperature rise.

2.1 Godiva-I Pulse Reactor Coupling Calculation and Validation

The Godiva-I pulse reactor was developed by Los Alamos National Laboratory (LANL) with a bare spherical geometry design without reflector. The fuel consists of metallic uranium with 93.8% enrichment, a fuel radius of 8.7407 cm, and a total loading of 52.42 kg of ^{235}U, exhibiting typical fast neutron spectrum characteristics [11][12]. Due to the extremely short operation time of the Godiva-I pulse reactor—a transient process on the microsecond scale—the average fuel temperature rise is 17 K. Within this small temperature rise range, property variations such as the thermal expansion coefficient (1.39$×10^{-5}$ K^{-1}) and thermal conductivity (27.5 $W \cdot m^{-1} \cdot K^{-1}$) of metallic uranium fuel are less than 1%, with geometric deformation dominating the reactivity feedback. Therefore, the constant property assumption adopted in ANSYS thermal-mechanical coupling calculations is reasonable. The material properties used in ANSYS calculations are listed in Table 1 [13][14].

The RMC and ANSYS models for the Godiva-I pulse reactor are shown in Figure 3 [Figure 3: see original paper]. RMC can receive temperature, density, and geometric dimension information output by ANSYS, while ANSYS can receive power distribution information output by RMC.

The RMC criticality calculation employs vacuum boundary conditions with 500,000 particles per generation, 150 inactive generations and 350 active generations, yielding an average standard deviation of approximately 0.000057.

Both ANSYS thermal analysis and mechanical calculations utilize transient solvers, with a total mesh count of approximately 170,000, total calculation time of 5.0$×10^{-4}$ s, time step of 5.0$×10^{-5}$ s, and 10 time steps. This study adopts the power at an initial period of 29.5 s as the total thermal power, with an initial temperature of 300 K for thermal analysis and adiabatic boundary conditions applied to the metal sphere surface. The mechanical calculation uses the temperature field generated from thermal analysis as the loading, with free expansion boundary conditions applied to the metal sphere surface and initial displacement set to zero.

Five iterative calculations were performed on the aforementioned model, with coupling parameters varying with iteration steps or time shown in Figure 4 [Figure 4: see original paper]. Figure 4a illustrates the convergence criterion keff variation during the iteration process, indicating that keff begins to converge from the 4th iteration, with the thermal-mechanical coupling calculation yielding a reactivity feedback of -0.0731 \$. The average temperature rise of the reactor is 17 K, therefore the fuel reactivity temperature coefficient is -0.0043 \$/K (1 \$ = 0.00645), with a relative deviation of -2.4% from the experimental value[12] of -0.0042 */K.Thereasonsforthecalculatedfuelreactivitytemperaturecoefficientbeinglowerthantheexperimentalvalue (a)theRMCmodelemploysvacuumboundaryconditionsonthespheresurface, failingtosimulateenvironmental to—many"mappingbetweenRMCcellsandANSYSmeshesresultsinaveragedfeedbackparameters, indirectlya averagedtemperatureriseandrelativevolumeexpansionversuspulsereactoroperationtimeobtainedfromANSY mechanicalcouplingcalculationsatiterationconvergence, wherethemaximumtemperatureriseiscalculatedas1* 3}$ cm, differing from literature values [3] by less than 1 m (3.5% relative deviation). The absolute deviations in temperature rise and displacement from literature values are minimal and do not significantly impact engineering evaluation of reactivity coefficients, thus these deviations can be neglected.

2.2 Godiva-IV Pulse Reactor Coupling Calculation and Validation

The Godiva-IV fast neutron pulse reactor employs a cylindrical fuel configuration, with the core model shown in Figure 5 [Figure 5: see original paper]. Godiva-IV features three equally spaced clamps holding a cylinder composed of highly enriched uranium and steel. The cylinder can be further decomposed into six fuel rings, with a main shaft and base screwed together to secure the fuel rings.

Each fuel ring consists of uranium with 93% ^{235}U enrichment alloyed with 1.5 wt% molybdenum. The rings contain three cylindrical blocks with compositions similar to the fuel rings. From top to bottom, these blocks are designated as the upper subassembly plate, middle subassembly plate, and safety block. Inside these components are the safety block base and main shaft, both made of stainless steel [2]. The main shaft and safety block base serve to hold the entire cylinder together. Similar to the Godiva-I pulse reactor, Godiva-IV operates on a microsecond timescale with an average fuel temperature rise of 49 K. Within this small temperature rise range, property variations such as the thermal expansion coefficient (1.48$×10^{-5}$ K^{-1}) and thermal conductivity (29.4 $W \cdot m^{-1} \cdot K^{-1}$) of the U-Mo alloy fuel are less than 2%, with geometric deformation dominating the reactivity feedback. Therefore, the constant property assumption adopted in ANSYS thermal-mechanical coupling calculations is reasonable. The material properties of the U-1.5%Mo alloy used in ANSYS calculations are listed in Table 2 .

As evident from the model description, the fuel rings, safety blocks, subassembly plates, and control rods are all composed of fuel material, and when assembled, they form a nearly gapless ring of highly enriched uranium. Therefore, for neutron transport calculations, it is unnecessary to retain all modeling details of the Godiva-IV model. The safety blocks, subassembly plates, and control rods are all treated as part of the fuel rings, while the C-clamps serving as fixtures are neglected to simplify the neutron transport model. The RMC coupling model includes six fuel rings (including corresponding portions of safety blocks, subassembly plates, and control rods), the main shaft, and the safety block base.

The ANSYS model requires detailed modeling, retaining details of gaps and free spaces, as gaps in the model may close or shrink during thermal expansion, thereby affecting component thermal expansion and thermal stress. The complete model includes six fuel rings, safety blocks, subassembly plates, control rods, main shaft, main shaft bolts, buffer pads, support pads, safety block base, safety block shims, C-clamps, and gaps between components. Figure 6 [Figure 6: see original paper] illustrates the RMC and ANSYS coupling models for Godiva-IV, with a total ANSYS mesh count of approximately 480,000.

The six fuel rings in the RMC model can respectively receive temperature, density, inner/outer radius changes, and height changes output by ANSYS. The RMC criticality calculation employs vacuum boundary conditions with 100,000 particles per generation, 150 inactive generations and 350 active generations, yielding an average standard deviation of approximately 0.000128.

The ANSYS thermal analysis calculation uses temperature measurements from fuel ring No. 4 and the safety block [2] as input loading, with air convection boundary conditions applied to all external surfaces. The mechanical calculation uses the temperature field generated from thermal analysis as loading, with boundary conditions set as fixed C-clamp centers and free expansion for all other components, and initial displacement set to zero.

Five iterative calculations were performed on the aforementioned model, with keff variation versus iteration steps shown in Figure 7 [Figure 7: see original paper]. The results indicate that neutronic-thermal-mechanical coupling converges at the 3rd iteration, with the converged keff taken as the average of iterations 3–5. Compared with the initial iteration, reactivity decreases by 0.1517 \$. The average temperature rise of the fuel rings is 49 K, therefore the fuel reactivity temperature coefficient is -0.003096 \$/K (1 \$ = 0.0065), with a relative deviation of -3.2% from the experimental value[15] of -0.003 \$/K. The reasons for the calculated fuel reactivity temperature coefficient being lower than the experimental value may include: (a) the RMC model employs vacuum boundary conditions on the sphere surface, failing to simulate environmental neutron reflection under experimental conditions, leading to overestimated neutron leakage rates; (b) although the ANSYS model retains fuel ring gaps, the RMC model simplifies the computational model and does not simulate gap closure at high temperatures, resulting in overestimated radial expansion and excessive negative reactivity feedback.

Figure 8 [Figure 8: see original paper] presents the temperature and displacement field contours obtained from ANSYS thermal-mechanical coupling calculations. The calculated maximum fuel temperature is 345 K, differing from literature values by 3 K (-0.87% relative deviation), and the calculated maximum fuel displacement is 1.26×10^{-2} cm, differing from literature values by 11 m (-8.7% relative deviation). The absolute deviations in temperature rise and displacement from literature values are minimal and do not significantly impact engineering evaluation of reactivity coefficients, thus these deviations can be neglected.

3 Feedback Effect Comparison

To investigate the impact of thermal expansion on reactivity, comparative studies were conducted by separately varying geometry and temperature. The corresponding fuel reactivity feedback coefficients were calculated and compared for two cases: considering temperature feedback only and considering both temperature and geometric expansion feedback, thereby determining the proportion of reactivity feedback contributed by thermal expansion effects to the overall core reactivity feedback.

Table 3 lists the fuel reactivity temperature coefficients calculated for the Godiva-I pulse reactor in the temperature range of 300 K to 317 K, considering temperature variation alone and simultaneously considering temperature and geometric changes. The results show that in the 300 K to 317 K temperature range, the reactivity feedback considering only the Doppler effect is -0.0031 \$. When both Doppler broadening and thermal expansion effects are considered, the negative reactivity feedback is -0.0731 \$. These results indicate that among the negative feedback effects caused by fuel temperature rise, approximately 95% originates from thermal expansion effects, while only about 5% comes from Doppler broadening effects.

Table 4 lists the fuel reactivity temperature coefficients calculated for the Godiva-IV pulse reactor in the temperature range of 292 K to 341 K, considering temperature variation alone and simultaneously considering temperature and geometric changes. The results show that in the 292 K to 341 K temperature range, the reactivity feedback considering only the Doppler effect is 0.0215 \$. When both Doppler broadening and thermal expansion effects are considered, the reactivity feedback is 0.1517 \$. These results indicate that among the negative feedback effects caused by fuel temperature rise, approximately 85% originates from thermal expansion effects, while only about 15% comes from Doppler broadening effects.

Table 3. Godiva-I feedback effect calculation results

State	keff	Reactivity Coefficient/(\$·K^{-1})	Literature [15]
Cold (300K)	0.99987±0.00006		
Hot (317 K) no expansion	0.99985±0.00006		
Hot (317 K) with expansion	0.99939±0.00006		

Table 4. Godiva-IV feedback effect calculation results

State	keff	Reactivity Coefficient/(·K^{-1})	Literature[15]
Cold(292K)	1.01821±0.00012		
Hot(341K) no expansion	1.01807±0.00012		
Hot(341K) with expansion	1.017		

Conclusion

This study developed a neutronic-thermal-mechanical coupling methodology centered on the RMC Monte Carlo neutron transport code and ANSYS finite element software. Through a closed-loop iterative framework of "power distribution → temperature/displacement fields → geometry/cross-section updates → neutron transport," the method achieves dynamic coupling of neutron physics, thermal-hydraulics, and structural mechanics. Neutronic-thermal-mechanical coupling calculations and fuel reactivity feedback coefficient validations were performed for both Godiva-I and Godiva-IV pulse reactors, and the relative contributions of thermal expansion and Doppler broadening to reactivity feedback were compared by separately varying geometry and temperature.

For the Godiva-I pulse reactor, the neutronic-thermal-mechanical coupling calculation yielded a fuel expansion reactivity temperature coefficient with a -2.4%

relative deviation from the experimental value; the calculated maximum fuel temperature rise differed from literature values by 1 K (6.25% relative deviation); and the calculated maximum fuel displacement differed from literature values by less than 1 m (3.5% relative deviation). For the Godiva-IV pulse reactor, the calculation yielded a fuel expansion reactivity temperature coefficient with a -3.2% relative deviation from the experimental value; the calculated maximum fuel temperature rise differed from literature values by 3 K (-0.87% relative deviation); and the calculated maximum displacement differed from literature values by 11 m (-8.7% relative deviation).

Comparative analysis of Doppler broadening and thermal expansion effects on reactivity feedback revealed that thermal expansion reactivity feedback dominates in both Godiva-I and Godiva-IV pulse reactors. The total reactivity feedback from Doppler broadening and thermal expansion in Godiva-I is approximately -0.0731 $, where thermal expansion accounts for 95% of the feedback effect. For Godiva-IV, the reactivity feedback from Doppler broadening and thermal expansion is approximately -0.1517 $, with thermal expansion accounting for 85% of the feedback effect. These results clearly demonstrate that geometric deformation induced by thermal expansion plays a decisive role in reactivity control in fast neutron pulse reactor systems, while the contribution of the traditionally significant Doppler effect is relatively minor in such compact metallic fuel reactors. This finding carries important implications for understanding the safety characteristics of fast reactor systems.

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Note: Figure translations are in progress. See original paper for figures.