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Neutronics and Thermal Hydraulic Coupling Analysis for MTR Reactors

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ABSTRACT

The integration of neutronics and thermal-hydraulic in multi-physics coupling analysis plays a crucial role in achieving high-fidelity simulations of nuclear reactor cores. In the current work, the neutronics and thermal hydraulic Multi-physics coupling methodology was proposed for the plate-type fuel assemblies inside Material Test Reactor cores. The coupling technique is based on the two-way and external coupling paradigms and accomplished using Monte Carlo Reactor analysis and sub-channel thermal-hydraulic codes. The coupling interface was developed using Python and Modern Fortran programming languages. The three-dimensional reactor physics modelling was developed using MCNP6 code while the one-dimensional thermal-hydraulic model was developed using PARET/ANL v2.1 for a typical Material Test Reactor (MTR) plate-type fuel reactor. Subsequently, the coupling analysis was conducted using the developed integrated code system. The simulation results from the coupling and non-coupling methods were compared to validate the feasibility of the coupling approach, revealing that the proposed coupling method offers greater accuracy compared to the traditional approach.

NOMENCLATURE

MTR	: Material Test Reactor
RR	: Research Reactor
ETRR-2	: Egypt Second Research Reactor
ENDF	: Evaluated Nuclear Data File
CRP	: Coordinated Research Projects
NK/TH	: Neutronic / thermal hydraulic

1. INTRODUCTION

Simulation of Research Reactors (RR) cores relies on detailed physical models with their inherent feedback mechanisms Utilizing advanced computational codes to accurately represent the intricate physics and to provide accurate estimates of system behavior.

Nuclear reactor analysis is particularly challenging, not only because of the complex physics and interdependent phenomena occurring within the reactor core but also due to the system's three-dimensional nature. Accurately estimating reactor safety parameters requires considering several interconnected phenomena, including neutron transport, heat transfer, fluid dynamics, and fuel performance… etc.

In a fission-based nuclear system, the neutron density (and, thus, the power) and the fluid conditions depend on each other. It is important to consider the interdependence between the different fields of the underlying physics. This is summarized in the schematics in Figure 1.

Reliable and accurate numerical simulation of these underlying complex physical phenomena requires a simultaneous description of several physics' components. Which requires computational high-fidelity multi-physics coupling of several different physics solvers [1].

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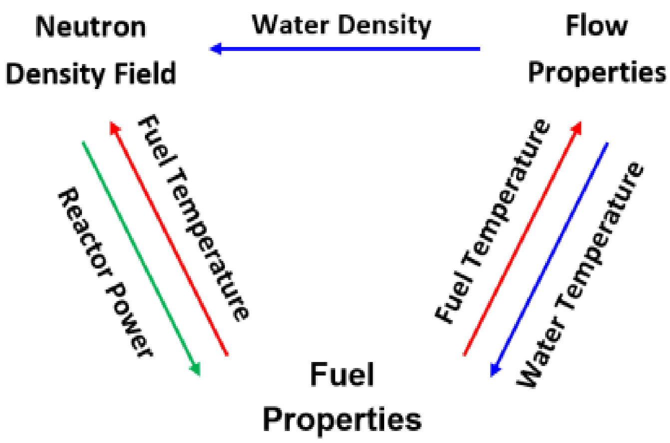

Fig. (1): Aspects of Multi-Physics Coupling in a Reactor Core

In the past, computation time had limited high-fidelity techniques to simplified models and limited their use as audit tools for less accurate methods [2]. Therefore, the researchers relied on one type of calculation, either thermal-hydraulic or neutronic. The following studies describe the calculations performed using standalone codes.

Tian et al. [3] developed a thermal-hydraulic analysis code for the China Advanced Research Reactor (CARR) to analyze plate-type fuel reactor cores. Their research investigated the heat transfer and flow distribution properties within the reactor core. Lu et al. [4] investigated the blockage accident in a single assembly channel of a 10 MW plate-type fuel reactor. The study revealed that the blockage led to a temperature increase in neighboring channels. Furthermore, it was observed that boiling occurred only in the hot channel of the obstructed assembly, as lateral heat conduction from adjacent channels helped mitigate boiling in other areas. Bousbia-Salah et al. [5] used the MCNP5 code to calculate the neutron flux and power distribution for a 10 MW MTR. Their results demonstrated that MCNP5 was a reliable tool for simulating the plate-type fuel core, with the calculated outcomes showing good agreement with a previous study. Xoubi et al. [6] explored how enrichment affects neutron flux in the in-core facility of a 10 MW MTR using OpenMC. Their study emphasized the critical role of flux trap calculations during the conversion of the reactor core from HEU to LEU.

While advancements in computing technology, particularly the availability of cost-effective computing resources, have significantly improved the overall efficiency of high-fidelity modeling, researchers have increasingly adopted the coupling method for more comprehensive analyses.

Linrong Ye et al. [7] coupled Fluent with Monte Carlo code through the UDF module to analyze a typical plate-type fuel assembly. Additionally, a fuel assembly blockage accident was analyzed using the proposed coupling code. The study indicated that with a 30% inlet blockage, the maximum coolant temperature increased by approximately 20°C, while the maximum fuel temperature rose by around 30°C. Zhiying Yue et al. [8] evaluated the performance of plate-type fuel by implementing a coupled calculation using the neutron physics code OpenMC, the fuel performance analysis code BEEs-Plates, and the nuclear reactor system analysis code NUSAC. The results indicated that the maximum fuel burnup would reach 16.91% FIMA after 240 days. As fuel burnup increases, the peak power of the fuel assembly shifts significantly towards the ends along the height direction. Additionally, the VonMises stress, volume stress, creep strain, and displacement of the fuel become substantial. Lastly, the effect of the coupled calculation on computational accuracy and efficiency was preliminarily examined. Xiaobei Xu et al. [9] developed a coupling code system named NECP-CLAMPERL, which integrates neutronics, thermal-hydraulics, and fuel performance. This system is built on the high-fidelity neutronics code NECP-X, the sub-channel thermal-hydraulics code CTF, the finite-element fuel performance code NECP-CALF, and the Multiphysics Object-Oriented Simulation Environment (MOOSE). The data transferred within the coupling system includes power, fuel temperature, clad surface temperature, coolant temperature, and density. The coupling method, based on Picard iterations, is combined with a predictor/corrector scheme to carry out depletion-dependent coupled simulations. The critical quantities such as power, reactivity, fuel temperature, and coolant temperature are selected to assess the convergence of the coupling iterations.

Building on these advancements, this study proposes a fully coupled neutronics and thermal-hydraulic analysis using MCNP6 [10] and PARET/ANL v2.1 [11, 12]. This integrated approach aims to realistically simulate the behavior of an MTR plate-type fuel research reactor. By analyzing a typical plate-type fuel assembly, the thermal-hydraulic and neutronics features were studied in detail, further emphasizing the utility of coupling codes in advancing the accuracy and reliability of reactor performance evaluations.

The results of the developed coupled analysis are compared to standalone simulations and the results from the past IAEA Coordinated Research Projects (CRPs 1496 and 2026).

The objective of CRP 1496 was to benchmark thermal-hydraulic and neutronic codes for research reactors using experimental data for the first time. It aimed to establish benchmark data, identify further research needs, compare results across organizations and codes, and assess user effects [13].

While the objective of CRP 2026 was to validate the computational models and codes needed for improving reactor design, operation, and safety, requiring benchmarking against experimental data. This task was done by collecting experimental data and evaluating computational methods for fuel burnup and material activation [14,15].

2. MODEL PREPARATION

2.1 Facility Description

The initial core of Egypt Second Research Reactor (ETRR-2), which is no longer in which was modified many times based on the operation history of ETRR-2, was selected for this study. ETRR-2 is a 22 MWth open pool reactor designed and manufactured by INVAP, moderated and cooled by forced upward circulation of light water. The original core comprised of 29 fuel elements of three types, differentiated by their U-235 mass content: Type 1 (~146 g), Type 2 (~209 g), and Standard (~404 g). Additionally, the core included a Cobalt Irradiation Device (CID) for Co-60 production. The reactor core configuration consisted of an array of fuel elements, reflectors, control plates, gadolinium injection boxes, and irradiation devices. Each fuel assembly was constructed with two aluminum side plates securing 19 fuel plates. These plates are composed of U3O8 powder enriched to 19.7% by weight of U-235, dispersed in an aluminum matrix with aluminum cladding [15,16].

Figure 2 illustrates the core configuration, while Table 1 provides general specifications of the ETRR-2 reactor core [16,17].

Table (1): Design specifications data of the ETRR-2 reactor [16].

Fuel material	U3O8
Uranium Enrichment (wt)	19.7%
Uranium U_3O_8 density (g/cm^3)	8.1
Fuel plate dimensions (cm)	84.0 ×7.0 × 0.150
Fuel plate active dimensions (cm)	80.0 × 6.4× 0.070
Cladding material	Al-6061
Density of cladding material (g/cm^3)	2.700
No. of control plates	6
Control plate material	Ag–In–Cd
Control plate cladding material	AISI 316 L
Control plate external dimensions (cm)	100 × 14.57 × 0.53
Control plate active dimensions (cm)	82.0 × 14.40 × 0.36
Reference pressure of the facility	0.2 MPa
Coolant (flow direction)	(upwards)
Water channel thickness between two fuel plates (cm)	0.270
Water channel thickness between two fuel elements (cm)	0.390
Moderator	Light water
Reflector	Beryllium
Max. heat flux (W/m^2)	1,170,000
Nominal flow rate (m^3/h)	1900

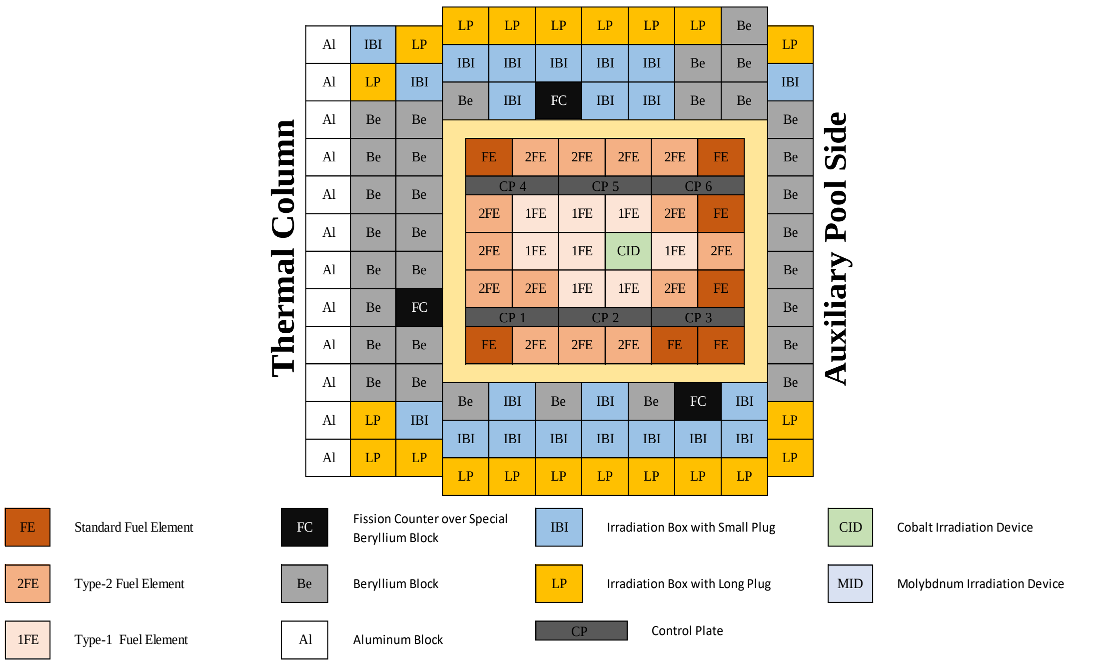

Fig. (2): Horizontal View of ETRR-2 Reactor First Core

2.2 Computational Codes

Two codes were used MCNP6 for Neutronics, and PARET/ANL v2.1 from the MTR/PC package for Thermal-Hydraulics.

MCNP6 code is a general-purpose, continuous-energy, generalized-geometry Monte Carlo transport code. This code has the capability of performing burnup calculations [10]. Evaluated Nuclear Data File (ENDF) version ENDF/B-VII.1 was used as the nuclear data library in this research.

The PARET/ANL v2.1 sub-channel code [11,12] has been utilized by the Reduced Enrichment Research and Test Reactor (RERTR) Program for transient and thermal-hydraulic analysis of research and test reactors with both plate-type and pin-type fuel assemblies. This version has undergone comprehensive validation through comparisons with the SPERT I and SPERT II experiments, covering both light water and heavy water systems. The Sub-channel codes are used for multi-component modeling in the core. A core is represented by the sub-assemblies and the sub-assembly by different sub-channels and other water channels and fuel rods. The time-dependent thermal energy balance equations are solved for control volumes in the scale of sub-channels [18].

The PARET code solves the governing time-dependent thermal energy balance equations describing the system after discretizion using finite-difference method in both space and time and subsequently solved numerically. It accommodates single-phase or two-phase coolant conditions. Reactor power is determined using the point-kinetics model, with feedback effects included based on changes in coolant temperature, moderator density, and fuel expansion. It simulates the fueled regions of a reactor core using a channel-based approach. The model allows for multiple independent channels, which interact only through reactivity feedback mechanisms affecting the entire core [11,12].

2.3 Numerical Modelling

ETRR-2 has been modeled using the reactor specifications for the original 29 fuel elements core described in Ref.[14, 15].

In the MCNP model, the axial cells were increased from 20 to 21 to match the number of axial nodes in PARET. The criticality calculation option (KCODE) was used to calculate the system's criticality. All nuclear cross-sections were recalled at a cold state (~20°C). A total of about 350 cycles of which 150 were skipped and 50000 histories per cycle were employed to reach a standard deviation of around 23 pcm.

In the PARET model, the core is represented by only two channels; for simplification, the first represents one fuel element while the second represents the remaining 28 fuel elements.

The result of the standalone simulations compared to the original models and the results from the past IAEA Coordinated Research Projects (CRPs) are shown in Table 2 and Table 3 respectively.

Table (2): Neutronics Result Validation – Standalone Simulation

	New Model	Original Model	CRP2026
K_{eff}	$1.06193 \pm 0.00023^{**}$ 5831.8 ± 23 pcm	$1.06154 \pm 0.00023^{*}$ 5797.2 ± 23 pcm	1.06825 (6388.9 pcm)$^{+}$ 1.06600 (6191.3 pcm)*

$^{+}$ Measured (Cold-State)
* Calculated (Cold-State) using WIMS5B/CITVAP, the difference between MCNP and WIMS5B/CITVAP should be less than 500 pcm.
** calculated (cold- state) using MCNP6.

Table (3): Thermal-Hydraulics Result Validation – Standalone Simulation

Maximum Temperature	New Model^{+}		CRP1496	
	Hot Channel*	Avg. Channel	Hot Channel	Avg. Channel
Fuel	110.0200	69.2830	--	--
Clad	107.3604	68.2280	--	--
Coolant	65.1458	49.9880	--	51.9**

* Calculated assuming 2.5 power peaking factor.
$^{+}$ Obtained from PARET.
** obtained from RELAP5 simulation at power 20.6 MW.

The missing values are due to the fact that they were not calculated in the CRP.

3. COUPLING METHODOLOGY

3.1 Model Nodalization and Data Exchange

The coupling process utilizes a one-dimensional representation of a fuel plate along the axial direction, assuming symmetry at the radial boundaries. In the thermal-hydraulic code, each node represents the boundary of a volume cell, whereas in the neutronics code, a node corresponds to the center point of a volume cell within a fuel plate or sub-channel. Figure 3 illustrates the axial nodalization for a single volume cell (fuel plate).

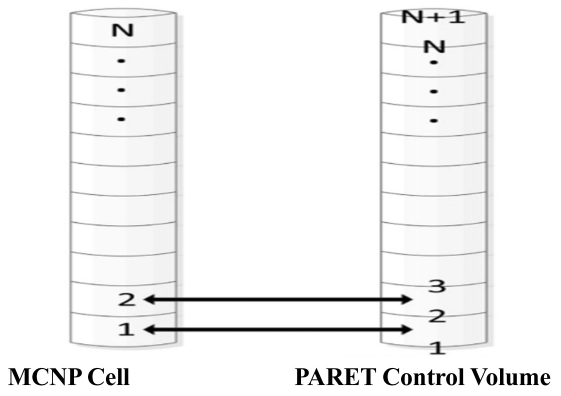

Fig. (3): Axial Representation for Data Exchange in the Coupled Code

At the first node (N=0) in the thermal-hydraulic code, the inlet boundary conditions for the coolant sub-channel are established. The geometric representation remains consistent between the PARET and MCNP6 codes. PARET outputs parameters such as temperature, density, pressure, and mass flux at the boundaries of each volume cell as a function of axial height. Meanwhile, MCNP6 provides power output at the center of each cell.

In total, 21 volume cells and 22 cell boundaries are defined, with quantities specified at the center of each cell. Figure 4 also illustrates the main parameters exchanged between the PARET and MCNP6 codes during the data transfer process.

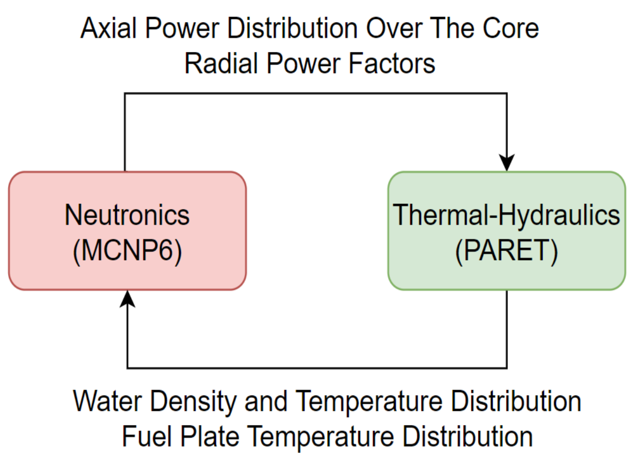

Fig. (4): Coupled MCNP6/PARET Data Transfer Procedure

3.2 MCNP Power Calculation

MCNP is utilized to simulate neutron particles and their average behavior within materials, where the particles are tracked using evaluated cross-section data from the ENDF/B-VII.1 library. The tracked neutron paths represent the neutron flux distribution and are processed track by track with reaction cross-sections and heating functions to calculate the estimated heating energy, corresponding to the power distribution [14,15]. In MCNP, the heating (power) distribution is directly calculated using either the F6 tally or the F7 tally. The F6 tally serves as a track-length estimator for energy deposition in a cell, while the F7 tally estimates fission energy deposition specifically in fissionable materials. In neutron-mode simulations, the F6 tally excludes gamma heating due to the absence of photon transport, whereas the F7 tally includes gamma heating since photons are deposited locally [14,15].

Both F6 and F7 are volume tallies that provide the average heating energy deposited within a volume cell of a fuel plate.

In this study, only F6 tally for both neutrons and photons are used to get the true heating energy in a cell coming from both fission neutrons and generated gamma rays. The true heating energy in MCNP is defined as shown in Equations (1) and (2).

$$\text{True Heating} = F_6{:}N + F_6{:}P \;\Rightarrow\; F_6{:}N,P \qquad \textbf{(1)}$$

$$F_6 = W_t . T_l . \sigma_{TOT}(E) . h(E) . \frac{\rho_a}{m_c} \qquad \textbf{(2)}$$

Where

F_6	:	Heating Energy (MeV/g)
W_t	:	Particle weight
T_l	:	Track length (cm)
$\sigma_{TOT}(E)$	:	Total microscopic cross section (barns)
$h(E)$	:	Heating number (MeV/collision)
ρ_a	:	The atom density (atoms/barn-cm)
m_c	:	mass of the cell (g)

Additionally, in this study, power conversion is made to be compatible with the PARET input format. So, the heating energy from MCNP (Power in MeV/g) is converted into (Relative Power) by using the following expression:

$$RP_{element,z} = \frac{e_{element,z}}{\left(\sum_{z=1}^{Z} e_{element} \Big/ Z\right)} \quad (3)$$

Where

$e_{element,z}$: The heating energy in Mev/g as a function of the axial height z,

Z : Total number of axial nodes, and

$RP_{element,z}$: Relative power as a function of the axial height.

3.3 PARET Temperature Distribution Procedure

PARET [16] employs point kinetics equation to compute reactor power and supports up to 15 groups of delayed neutron data. For this study, six groups of delayed neutron data were utilized. The total reactor power is determined in PARET using the following equations.

$$\frac{dP(t)}{dt} = \frac{\rho(t) - \beta}{\Lambda} P(t) + \sum_{i=1}^{n} \lambda_i C_i(t) + S(t) \quad (4)$$

$$\frac{dC(t)}{dt} = \frac{\beta f_i}{\Lambda} P(t) - \lambda_i C_i(t) \quad (5)$$

Where

$\rho(t)$: the reactivity of the system as a function of time,

β : the effective delayed neutron fraction,

Λ : the prompt neutron generation time,

λ_i : decay constant for group i,

C_i : concentration of delayed neutron precursors of group i,

f_i : the fraction of delayed neutrons of group I,

β_i/β, and $P(t)$is the reactor power as a function of time.

PARET uses conservation of energy, mass, and momentum equations as shown below.

$$\rho'' \frac{\partial E}{\partial t} + G \frac{\partial E}{\partial z} = q \quad (6)$$

$$\frac{\partial \bar{\rho}}{\partial t} = -\frac{\partial G}{\partial z} \quad (7)$$

$$\frac{\partial G}{\partial t} + \frac{\partial}{\partial z}\left(\frac{G^2}{\rho'}\right) = -\frac{\partial p}{\partial z} - \left(\frac{f}{\rho}\right)\left(\frac{|G|G}{2D_e}\right) - \bar{\rho} g \quad (8)$$

Where

$$\bar{\rho} = \rho_l(1-\alpha) + \rho_v \alpha \quad (9)$$

$$\frac{1}{\rho'} = \frac{(1-x^2)}{\rho_l(1-\alpha)} + \frac{x^2}{\rho_v \alpha} \quad (10)$$

$$\rho'' = [\rho_l x + \rho_v(1-x)] \frac{\partial \alpha}{\partial x} \quad (11)$$

Where

G : the mass flow rate,

p : the pressure,

E : the enthalpy,

f : the friction factor,

D_e : the equivalent hydraulic diameter,

ρ : the average density,

ρ' : momentum density,

ρ'' : the slip flow density,

x : the vapor weight fraction (quality),

α : the vapor volume fraction (void fraction).

The heat transfer model in PARET is based on a one-dimensional conduction solution, which limits heat conduction to the cladding and coolant channel. Heat transfer within the fuel plates is calculated by solving the one-dimensional conduction equation in the radial direction.

$$\frac{\partial(\rho c_p T)}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + f_s S \quad (12)$$

Where

T : the temperature,

x : the radial coordinate,

ρc_p : the volumetric heat capacity,

k : the thermal conductivity,

S : the heat source per unit volume,

f_s : heat source flag such that in $f_s = 1$ in the fuel meat and $f_s = 0$ in the clad.

Axial heat conduction along the fuel plate length is neglected in the PARET model, as it is assumed that all the heat generated travels across the cladding/coolant interface. A key component of the heat conduction solution is calculating the convective heat transfer coefficient. To achieve this, PARET incorporates thermal hydraulic correlations to determine the heat transfer coefficients in each heat transfer regime.

3.4 Coupling Procedure

MCNP6 and PARET were coupled using explicit, external, loose coupling and serial integration of multi-physics modules into a united multi-physics system by developed Fortran routines the control the data exchange while Python script was used as a driver for the whole process, data post-processing and data visualization. Also, they were coupled through the distribution of heating energy ("power") in the fuel plate as a function of axial height (z), represented by e_z from the MCNP simulation, alongside water density and temperature distributions in the flow sub-channel, denoted by $\rho_w(z)$ and $T_w(z)$, respectively.

Additionally, the average fuel and cladding temperature distributions in the fuel plate, denoted by $T_F(z)$ and $T_C(z)$ from the PARET simulation, were also used.

The coupling interface consists of abstract Fortran routines responsible for pre-defined tasks. The major tasks cover coupling initializing, running the standalone models in a serial scheme, saving the date, updating the data with the right format for each code, generating coarse temperature-dependent neutron cross-sections, and checking the convergence of the resulting data. Furthermore, a Python script was developed to pros-process the converged data, extract the parameters required for the assessment and finally for data visualization.

4. RESULTS AND DISCUSSION

A coupled analysis was conducted using the ETRR-2 model to evaluate the convergence of the coupling procedure. The MCNP calculations were constrained to 350 cycles with 50,000 particles per cycle due to the significant computational time required, primarily by MCNP.

The result of the coupled simulations of the two codes compared to the standalone simulation at a hot full power are shown in Table 4 and Table 5 respectively. The ETRR-2 reactor lacks neutronics and thermal-hydraulics measurements under hot full power conditions.

Table (4): Neutronics Result Validation – Coupled Simulation

	Coupled Model*	Standalone Model
K_{eff}	1.05997 ± 0.00023	1.06193 ± 0.00023

* Calculated (Hot-State)

The results of the coupled simulation align with expectations, as the available neutron population (i.e., excess reactivity) is expected to decrease in the hot state with xenon poisoning compared to the cold state. Since the standalone code calculates reactivity assuming a constant low temperature corresponding to the cold state, the coupled approach provides a more realistic representation of reactor behavior under operating conditions.

Table (5): Thermal-Hydraulics Result Validation – Coupled Simulation

Maximum Temperature	Coupled		Standalone Model	
	Hot Channel+	Avg. Channel	Hot Channel*	Avg. Channel
Fuel	117.4610	76.7421	110.0200	69.2830
Clad	111.5723	74.9852	107.3604	68.2280
Coolant	65.2130	50.0120	65.1458	49.9880

* Calculated assuming 2.5 power peaking factor.

\+ Calculated a power peaking factor of 2.18 after convergence of 7 iterations.

Similarly, the thermal results obtained from the coupled simulation are consistent with expectations. The coupled model accounts for the increase in coolant temperature during operation, reflecting a dynamic thermal response rather than assuming a constant temperature. In contrast, the standalone code assumes a fixed temperature, leading to lower thermal values. As a result, the coupled simulation provides a more accurate and realistic representation of the reactor's thermal behavior

CONCLUSION

In conclusion, this study demonstrates the successful development and implementation of a coupled Neutronics/Thermal-Hydraulics system using MCNP6 and PARET for research reactor analysis. The automated coupling procedure allows for accurate simulations of reactor power distribution, thermal-hydraulic properties, and temperature profiles, ensuring a more realistic representation of reactor behavior. The system was validated through comparison with standalone Neutronics and Thermal-Hydraulics simulations, as well as benchmarks from previous CRPs. The coupled procedure proved effective in achieving convergence within seven iterations, despite challenges related to particle statistics in MCNP. The results highlight the importance of coupling these models to improve accuracy and provide a deeper understanding of reactor performance under various operating conditions. Future work should focus on enhancing particle statistics to further reduce uncertainties and expand the applicability of the coupled system to other reactor types.

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