SENG 492 Senior Project

MedicalAI

Multidisciplinary Delivery Assesment Analysis

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Introduction

The accurate analysis of nuclear reactors requires the integration of two core disciplines: thermal-hydraulics and neutronics. Thermal-hydraulics governs the behavior of fluids within the reactor, influencing temperature, velocity, and pressure fields, while neutronics focuses on neutron behavior and fission reactions. Traditionally, these domains are examined independently. However, in practice, they are tightly coupled. For instance, neutron flux directly drives heat generation via fission reactions, which alters local temperatures and fluid properties; in turn, these thermal conditions impact neutron cross-sections and moderation characteristics.

In this study, they develop a comprehensive multiphysics model that couples thermal-hydraulic and neutronic analyses using ANSYS Fluent. The reactor geometry is modeled as a simplified channel within which these interactions occur. Neutron diffusion equations, representing both fast and thermal groups, are incorporated into the CFD environment using User Defined Scalars (UDS), while associated material behaviors and source terms are coded via User Defined Functions (UDFs). This setup allows for bidirectional feedback: thermal-hydraulic conditions affect neutron behavior, and neutron fluxes determine heat generation profiles, thereby influencing fluid dynamics in subsequent iterations.

This integrated approach was applied first to a Pressurized Water Reactor (PWR) as a baseline case, and then extended to a Molten Salt Breeder Reactor (MSBR) — a more complex Generation IV concept. The outcome is a coupled and iterative analysis system capable of modeling real-time physics-based interactions within reactor systems.

2. Multidisciplinary Approach

Although the foundation of this project lies in nuclear engineering, its successful execution demanded a combination of expertise across multiple scientific and engineering domains. This holistic methodology was necessary to effectively model the complex physical phenomena within nuclear reactors, especially under coupled multiphysics conditions.

- **Mechanical Engineering:** The application of Computational Fluid Dynamics (CFD) was essential to simulate the behavior of coolant flow within the reactor channel. Using ANSYS Fluent's solvers, detailed models of velocity, pressure, and temperature distributions were obtained. These thermal-hydraulic parameters played a vital role in influencing neutron behavior.
- **Applied Mathematics & Physics:** The modeling of neutron transport required the formulation and implementation of the two-group neutron diffusion equations. These partial differential equations (PDEs) describe the spatial and energy-dependent flux of neutrons and were implemented in a way that allowed them to interact dynamically with thermal-hydraulic parameters.
- **Software and Computational Engineering**: One of the most technically demanding aspects was integrating custom physics into ANSYS Fluent using User Defined Functions (UDFs) and User Defined Scalars (UDS). UDFs coded in C were used to define neutron source terms, absorption, scattering, and diffusion coefficients, while UDSs enabled Fluent to treat neutron fluxes as field variables that evolve throughout the simulation domain. Adjustments to keff (effective multiplication factor) and normalization schemes were managed using dedicated DEFINE_ADJUST routines.

This convergence of disciplines enabled the simulation of physically accurate interactions between the reactor's thermal and neutronic behaviors. Without the integration of these diverse fields, the project would not have been able to capture the complexity and feedback mechanisms inherent to real-world reactor operation.

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3. Reactor Types Modeled

In this study, two different reactor types were modeled and analyzed to validate the coupling methodology and explore its applicability across different reactor designs:

3.1 Pressurized Water Reactor (PWR)

The Pressurized Water Reactor is one of the most established and widely used types of nuclear reactors globally. Its thermal-neutronic behavior is well-documented, making it an ideal candidate for validation.

In their simulation, they modeled a simplified channel of a PWR core and used reliable cross-section data from literature. The neutron transport within the fuel and moderator regions was governed by two-group neutron diffusion equations, accounting for fast and thermal neutron interactions. Custom UDFs were written to define:

- Neutron source terms in fuel and moderator regions
- Group-wise diffusion coefficients (D1_F, D2_F, D1_M, D2_M)
- Cross-sections for absorption, fission, and scattering (e.g., SIGMA_A1_F, NU_SIGMA_F2)

They implemented these equations using User Defined Scalars (UDS) to represent the fast and thermal neutron fluxes, and their spatial evolution was monitored during the simulation. The keff (effective multiplication factor) was dynamically updated, and flux normalization ensured numerical stability. The goal of this phase was to ensure that our methodology reproduced expected results in a known environment.

3.2 Molten Salt Breeder Reactor (MSBR)

Following the successful implementation of the PWR model, they extended the simulation framework to the Molten Salt Breeder Reactor (MSBR), a Generation IV reactor concept characterized by its use of liquid fuel and unique thermal-hydraulic and neutronic properties. Unlike solid-fueled reactors, MSBR systems involve continuous circulation of fissile material, which introduces different flow and moderation characteristics.

They revised our UDFs to reflect the new cross-section parameters specific to MSBR designs**:**

- Modified fission and absorption rates for fast and thermal groups
- Inclusion of upscattering effects and removal cross-sections (e.g., SIGMA_R1_F, SIGMA_S21_M)
- Updated diffusion coefficients for both fuel and moderator materials

In this reactor, due to higher neutron moderation and different fluid properties, the flux distribution and keff behavior showed notable divergence compared to the PWR case. The MSBR model served as a testbed to validate the flexibility of our coupling framework and the robustness of our code under less conventional reactor conditions.

Through the simulation of both reactor types, they demonstrated the versatility and accuracy of our multiphysics framework. The distinct characteristics of each reactor provided insight into how thermal and neutronic feedback mechanisms manifest under different engineering constraints and design philosophies.

4. Multiphysics Coupling Logic

The primary objective of this study is to enable two-way coupling between thermal-hydraulic and neutronic physics within ANSYS Fluent to emulate the interdependent behavior found in real nuclear reactors. This was achieved by designing a simulation environment where outputs from one physical model become inputs to the other in an iterative loop.

The coupling strategy operates on the following principles:

- **Thermal-to-Neutronic Feedback**: Temperature fields generated from CFD simulations directly influence neutron behavior. For example, rising temperatures reduce moderator density, which in turn alters the moderation ratio and neutron flux spectrum. These temperature-dependent properties (e.g., macroscopic cross-sections) were integrated via temperature-sensitive functions within the UDFs.
- **Neutronic-to-Thermal Feedback**: Neutron fluxes determine local heat generation through fission reactions. The UDS-defined neutron flux values were used to compute the volumetric heat source terms in the fluid domain. These source terms then contributed to energy equations, completing the feedback loop.
- **Iterative Loop Structure**: The simulation workflow follows an iterative procedure:
    1. Initialize velocity, pressure, and temperature fields.
    2. Solve for neutron fluxes using current thermal parameters.
    3. Calculate new heat generation rates.
    4. Update energy and momentum equations.
    5. Repeat until convergence is reached for all coupled variables.

This bidirectional feedback mechanism mirrors the actual operational dynamics of nuclear systems and allows for more accurate prediction of reactor performance, especially under transient or extreme conditions.

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5. Implementation in ANSYS Fluent

The implementation of this multi-physics model within ANSYS Fluent relied heavily on its extendable architecture through User Defined Functions (UDFs) and User Defined Scalars (UDS).

5.1 User Defined Scalars (UDS)

To represent the neutron fluxes as physical field variables, two UDSs were introduced:

- One for fast neutron flux
- One for thermal neutron flux

These scalars were treated as passive scalars within Fluent but were solved using custom source and diffusion terms to represent the two-group neutron diffusion equations. This allowed for spatial and temporal tracking of neutron population behavior within the reactor domain.

5.2 User Defined Functions (UDF)

C-based UDFs were written to define:

- Source terms for each neutron group based on fission, scattering, and absorption processes.
- Spatially dependent diffusion coefficients.
- Temperature and material-dependent cross-sections (e.g., as functions of local temperature or velocity).
- Adjustments to normalization and criticality calculations via DEFINE_ADJUST.

Each reactor type had a dedicated set of UDFs:

- The **PWR UDF** set used static parameters sourced from literature and was primarily used to validate the mathematical implementation.
- The **MSBR UDF** set accounted for more complex physics, including moving fuel, dynamic reactivity changes, and more fluid interaction between the fuel and moderator zones.

5.3 Setup Process

- UDSs were defined and initialized from the Fluent GUI.
- Custom UDFs were compiled and loaded into Fluent.
- Boundary and operating conditions were applied.
- Monitoring and convergence criteria were tailored to track both thermal-hydraulic and neutronic variables.

This modular design allows for reusability and flexibility. Future expansion of this framework could include additional physics, such as structural deformation or burn-up calculations.

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6. Validation and Verification

To ensure the accuracy and reliability of the implemented multi-physics coupling framework, a validation step was conducted using the Pressurized Water Reactor (PWR) model. The simulation results were compared with established benchmark data from literature.

The keff (effective multiplication factor) obtained from the Fluent-based simulation was 1.004, which is within 1% of the reference value of 0.996 for the selected configuration. Neutron flux distributions and temperature profiles were also qualitatively compared to those reported in prior studies, confirming the expected behavior and distribution trends.

Additionally, mesh sensitivity analysis was performed to ensure numerical stability. Convergence criteria were strictly enforced for both thermal and neutronic residuals, with all simulations achieving steady-state convergence within acceptable tolerance limits.

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7. Results and Visualization

7.1 PWR Results

- **Temperature Distribution**: The coolant reached peak temperatures in the mid-channel region, consistent with heat generation from neutron fission zones.
- **Neutron Flux Distribution**: Fast neutron flux peaked near the center of the fuel region, while thermal flux showed a more dispersed profile due to moderation effects.
- **Velocity Profiles**: The flow was parabolic, indicating a fully developed laminar regime, which aligns with the assumptions made in simplified channel modeling.

7.2 MSBR Results

- **Flux Distribution Changes**: Compared to the PWR, the MSBR showed a broader thermal flux distribution due to higher moderation and the fluid nature of the fuel.
- **keff Trends**: The effective multiplication factor varied more significantly due to the dynamic interaction between flowing fuel and temperature-dependent cross-sections.
- **Heat Generation Profile**: The source term adapted to spatial flux variations, resulting in non-uniform but physically consistent heating zones.

Color contour plots were generated in Fluent to visualize temperature, velocity, and neutron flux distributions for both cases. These visual tools were critical in validating the physical realism of the simulations.

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8. Challenges and Limitations

Implementing a coupled thermal-hydraulic and neutronic model within ANSYS Fluent presented several challenges:

- **Convergence Stability**: Simultaneous solution of coupled PDEs (momentum, energy, and neutron diffusion) occasionally led to numerical instability, especially in the MSBR case due to strong feedback loops.
- **Cross-section Data Sensitivity**: Accurate modeling required temperature-dependent cross-sections, which were only available for certain materials, limiting realism in some cases.

- **Geometry Simplification**: The use of a 2D or simplified channel geometry, while sufficient for validation, does not capture full 3D reactor behavior.
- **Scalability**: The UDF and UDS structure works well for small to moderate-size problems but may not scale efficiently for full-core simulations.

Conclusion

This multidisciplinary project successfully demonstrates the *feasibility and advantages of* performing coupled thermal-hydraulic and neutronic analyses within ANSYS Fluent. By extending the software with User Defined Scalars and Functions, they effectively embedded neutron diffusion physics into a CFD platform. This approach eliminates the need for external neutronics solvers and facilitates tightly integrated simulations.

Through modeling of both a traditional Pressurized Water Reactor and a Generation IV Molten Salt Breeder Reactor, the robustness of our coupling methodology was validated under different design conditions. The bidirectional feedback loop, essential for capturing real reactor behavior, was implemented and shown to impact both neutron distribution and thermal fields meaningfully.

The success of this study opens up new possibilities for real-time multiphysics simulations in reactor design and safety analysis. With further development, such as coupling with structural or chemical modules, the framework could become a valuable tool for next-generation nuclear engineering solutions.

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