

Identification of plausible phenomena for potential advanced fuel design using LLM

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1. Introduction

Within the top-down approach of fuel qualification for advanced reactors (NUREG-2246), it becomes more important to understand the fuel failure and degradation mechanisms. Phenomena Identification and Ranking Tables is one of the methodologies to identify governing mechanisms and play an important role in the Accelerated Fuel Qualification (AFQ) process [1]. As PIRT relies on the knowledge and opinions of experts, a methodology of PIRT based on literature has been proposed to avoid any possible distortion in the results of PIRT [2].

There have been studies conducted using text-mining and Large Language Model (LLM) agents, GPT, for PIRT. While the methodology using text-mining showed limitations in justifications [3], the results from LLM agents showed strong reasoning with minor hallucination [4]. However, both studies mainly focused on the capabilities of the methodologies, rather than the underlying the behavior of reactor systems.

In this study, text-mining and LLM have been adopted to collect the plausible phenomena of a fuel design example for Small Modular Reactors (SMRs). By introducing fuel failures criteria that are originated from section 4.2 of NUREG-0800, the PIRT table has been checked for its preparedness of sufficient phenomena.

2. Methods and Results

2.1 A Fuel Design Example

A fuel design example that is subject to PIRT in this study is assumed as below (Table 1). The example has been chosen to gather literature for PIRT. As it has been tested in Fast Flux Test Facility (FFTF), the legacy data on T91 is available and selected as cladding of the fuel.

Table 1. Design Overview

Component	Design
Reactor	Sodium-cooled Fast Reactor
Fuel slug	U-10Zr
Cladding	T91
Bonding	Sodium

2.2 A Table of Fuel Failure Modes

When collecting literature, it is ambiguous how much data is sufficient for identifying the phenomena for PIRT. As the experiences from licensing fuel designs of LWRs are reflected in NUREG-2246 (Fuel Qualification for Advanced Reactors), the main goals from NUREG-2246 are closely related to the criteria of 4.2 of NUREG-0800 which contains diverse failure modes with specific criteria. These failures are good examples resulting from governing phenomena which affect the main goals. This study utilizes the failures described in section 4.2 Fuel System Design of NUREG-0800 (Standard Review Plan) as candidates of fuel failure modes for the new fuel design. The categorization of failure modes is used as a base line for checking the sufficiency of the collected phenomena.

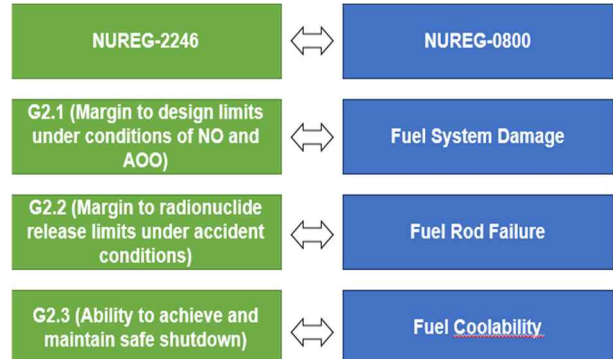


Fig 1. Main goals of NUREG-2246 and SRP criteria in 4.2 of NUREG-0800

2.3 Model Overview

For identifying phenomena subject to PIRT, this study introduces a methodology that consists of 5 steps, collection, integrating, extracting, refining and matching.

The abstracts of 593 papers were collected from SCOPUS via SCOPUS API and OSTI using keywords ("T91" OR "9Cr-1Mo" for the cladding, "U-10Zr" OR "U-Zr" for the slug) AND ("sodium" OR "fast reactor" OR "SFR") AND ("degradation" OR "damage" OR "failure" OR "interaction" OR "irradiation"). Then, the papers were checked for duplicate papers based on DOI number and similarity of titles and integrated to a total of 445 abstracts.

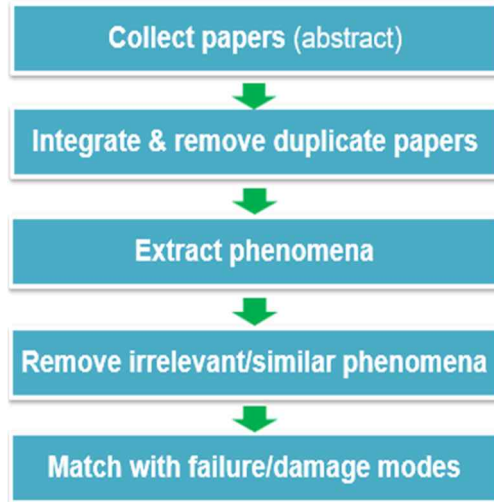


Fig 2. Process Diagram

To extract phenomena from the literature, texts were embedded with GPT (text-embedding-3-small) and clustered. This study used the concept of BERTopic for clustering. BERTopic is one of the topic modeling techniques that extract topic representation [5]. First, texts were converted to embedding representation using GPT and then downsized its dimensionality before clustering. The reduced embeddings are clustered by HDBSCAN, the density-based clustering. Density-based approach is particularly efficient for identifying clusters with complicated shapes and noise [6]. Then, the topic representation words were extracted based on the term frequency and inverse document frequency. The 15 topic representation words were given to GPT-4o with sample paper abstracts to generate the phenomena with few shots. However, some phenomena may haven't been studied frequently regardless of its importance. Thus, the noise clusters were also went through the same process as main clusters did.

The extracted phenomena were refined with GPT-4o to remove some irrelevant and similar phenomena with contexts (reactor type, fuel design overview) and mapped with failure modes by GPT-4o with few shots and descriptions of failure modes, allowing multiple mapping of phenomena with failure modes.

2.4 Results

The 13 phenomena have been mapped with 20 failure modes. As the repeated mapping results were inconsistent, the final results were organized only for cases where it was mapped 3 or more times out of 5.

For the failure modes regarding fuel system damage (Table 2), the fretting wear at contact points with no match showed insufficiency of collected literature because potential contact with wire wrap can cause wear, even though the impact may be insignificant. On the other hand, it is expected to have no match with "Hydraulic loads over holddown capability of fuel assembly" and "Control rod reactivity and insertability"

due to its inapplicability to SFR and absence of design features of control rods in the given contexts.

Table 2. Mapping results for fuel system damage

Failure modes	Phenomena
Stress, strain or loading for fuel system structural member over limits	- Creep-fatigue interaction - Fuel cladding mechanical interaction
Cumulative strain fatigue cycles exceeding design fatigue lifetime	- Creep-fatigue interaction
Fretting wear at contact points	N/A
Oxidation and the buildup of corrosion products	- Liquid metal corrosion - Fuel cladding chemical interaction
Dimensional changes	- Void swelling - Irradiation creep - Fuel swelling - Constituent redistribution - Radiation-induced microstructure evolution
Fuel rod internal gas pressure over nominal system pressure	- Fission gas diffusion - Fission gas release - Fuel swelling
Hydraulic loads over holddown capability of fuel assembly	N/A
Control rod reactivity and insertability	N/A

For fuel rod failure criteria (Table 3), as the keywords for collecting abstracts focused on the degradation of nuclear materials, thermohydraulic phenomena have been missed and unmatched with "Overheating of cladding", "Overheating of fuel pin" and "Excessive fuel enthalpy". Since "Cladding collapse" is not likely to happen in metallic fuel systems, no match result doesn't imply shortage of literature.

Table 3. Mapping results for fuel rod failure

Failure modes	Phenomena
Cladding collapse	N/A
Overheating of cladding	N/A
Overheating of fuel pin	N/A
Excessive fuel enthalpy	N/A
Pellet-Cladding interaction	- Fuel cladding chemical interaction - Constituent redistribution - Eutectic formation
Bursting	- Fission gas release - Fission gas diffusion
Mechanical Fracturing	- Irradiation embrittlement

With regard to fuel coolability criteria (Table 4), the "Violent expulsion of fuel" has no match because it is more relevant to thermohydraulic phenomena. The term "Fuel rod ballooning" is usually used in ceramic fuels. If

it should be used in SFR, it has to be modified to the term (e.g. fuel swelling) commonly used in metal fuels. As “Structural deformation” requires thermohydraulic and seismic analyses, there were no matched phenomena that were collected with keywords related to material degradation. “Eutectic formation” was mapped with “Generalized cladding melting” because the description of the failure mode includes beyond design basis conditions. The shortage of mapping capability has been observed in failure mode of “Cladding embrittlement” because it missed “Irradiation embrittlement”, the phenomenon.

Table 4. Mapping results for fuel coolability

Failure modes	Phenomena
Cladding Embrittlement	- Radiation-induced microstructure evolution
Violent expulsion of fuel	N/A
Generalized Cladding Melting	- Eutectic formation
Fuel Rod Ballooning	N/A
Structural deformation	N/A

3. Conclusions

This study proposed the methodology to identify the plausible phenomena for PIRT and check for its sufficiency using LLM and existing deterministic framework of fuel qualification. As the supplementary tool to develop the PIRT table for new fuel designs of advanced reactors, potential phenomena can be discovered by collecting and clustering the literature. The list of phenomena was mapped with failure modes of typical LWR fuels described in section 4.2 of NUREG-0800 as a basis to identify the missing parts for demonstration of fuel qualification required based on NUREG-2246.

However, keywords for collecting literature were mainly concentrated on material degradation aspects and insufficient to cover thermohydraulic failure modes which exist in criteria of NUREG-0800. In addition, some failure modes require modification based on its design features. Also, mapping capability showed deficiency that may require fine-tuning instead of few shots. Further research is required to improve the capability and optimize the model for diverse advanced reactor and fuel systems.

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