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Uncertainty & Sensitivity Analysis of Nuclear Fuel Using Transuranus & Dakota

UDYANTH VAIDYA

KTH Royal Institute of Technology

School of Engineering Sciences

Department of Physics

MSc in Nuclear Energy Engineering

KTH ROYAL INSTITUTE OF TECHNOLOGY
SCHOOL OF ENGINEERING SCIENCES

ABSTRACT

With the initiative taken by the SUNRISE project (Sustainable Nuclear Energy Research in Sweden) to construct a Lead-cooled research reactor, this thesis intends to extend the knowledge within nuclear fuel development. By using integral iterative modelling and simulating techniques that mimic real-world phenomena, novel fuel materials like uranium nitride are assessed for future validation.

The work deals with the fuel performance analysis of the SUNRISE LFR, employing the TRANSURANUS fuel performance code. This code contains a collection of model parameters that simulate the thermo-mechanical behaviour of the fuel cladding system on an engineering scale of the reactor core. A comparative study is performed for UO_2 and UN fuels using the same input data such as fuel geometry. In addition, predefined information relating to the neutronics analysis for the reactor was used as input to the TRANSURANUS code along with literature reviews to select the accurate models on the reactor, fuel, and its behaviour. Furthermore, a sensitivity study is carried out to assess the models and parameters affected by more significant uncertainty.

The uncertainty analysis of the UN fuel's swelling models is performed using the Dakota toolkit. The sampling of input data using the Dakota software coupled with the nuclear simulation program TRANSURANUS produced partial rank correlation coefficients significant to the modelling. However, since the assessed models displayed the same correlation coefficients, the results conclude that a deeper understanding of the theoretical swelling model might be required.

SAMMANFATTNING

I samverkan med initiativet av SUNRISEprojektet (Sustainable Nuclear Energy Research in Sweden) som syftar att bygga en blykyld forskningsreaktor, avser denna avhandling att utöka kunskapen inom kärnbränsleutveckling. Med användning av integral iterativ modellering och simuleringstekniker som efterliknar verkliga fenomen bedöms nya bränslematerial som uranmononitrid för framtida validering.

Arbetet behandlar analysen av bränsleprestanda för SUNRISE LFR, med användning av TRANSURANUS bränsleprestandakod. Denna kod innehåller en samling modellparametrar som simulerar det termomekaniska beteendet hos bränslebetäckningssystemet i en teknisk skala för reaktorkärnan. En jämförande studie utförs för UO2 och UN-bränslen med samma ingångsdata som t.ex bränslegeometrin. Dessutom användes fördefinierad information om den neutroniska analysen för reaktorn som ingångsdata till TRANSURANUSkoden tillsammans med granskning av litteratur för att välja lämpliga modeller för reaktorn, bränslet och dess beteende. Därtill genomfördes en känslighetsstudie för att bedöma de modeller och parametrar som påverkas av mer betydande osäkerhet.

Osäkerhetsanalysen av UN-bränslets svällningsmodeller utförs med hjälp av Dakota-verktyget. Samlingen
av indata med Dakota-programmet i kombination med kärnkraftssimuleringsprogrammet TRANSURANUS gav korrelationskoefficienter för partiell rang viktiga för modelleringen. Eftersom de utvärderade modellerna visade samma korrelationskoefficienter, tyder slutsatsen på att en djupare förståelse av den teoretiska svällningsmodellen krävs

ACKNOWLEDGEMENT

This degree project will conclude my two-year journey at KTH as a Master's Student. The thesis work presented me with many new learning possibilities and challenges that I am grateful for as the experience has developed me significantly. I would like to sincerely thank my supervisor Dr. Denise Adorno Lopes, who has supported me throughout this project and making the thesis more interesting with constructive feedback. I would also like to thank Dr. Janne Wallenius and Dr. Pär Olsson for giving me this opportunity to work on the SUNRISE project. Special Thanks to Dr. Jan Dufek, who was always supportive during my entire master's program here at KTH, without whom none of this would be possible. I also express my gratitude to all my Professors and lecturers at KTH that made this learning curve possible.

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LIST OF ACRONYMS	
BOL	Beginning of life
CDF	Cumulative damage function
EOL	End of life
FBR	Fast Breeder Reactor
FCT	fuel Centre Temperature
FGR	Fission Gas Release
FPC	Fuel performance codes
GIF	Generation IV international Forum
LFR	Lead Cooled Fast Reactor
LHS	latin hyper cube
PCMI	Pellet cladding mechanical interaction
SUNRISE	Sustainable Nuclear Research in Sweden
TU	TRANSURANUS

1 INTRODUCTION

With the ever-increasing population, a subsequent increase in the electricity demand and the recent trends in global warming have slightly aligned the stars for the nuclear power sector as international pressure is applied to countries to reduce greenhouse gas emissions. Many developing countries that rely on fossil fuel electricity generation are now obligated to look for an alternative. Although the negative externality of carbon emission is primarily absent from nuclear power, the dire consequences of major historical accidents serve as a good reminder of the unique disasters that can be caused by nuclear power. Hence, to bridge the gap with a culture of safety and public acceptance for nuclear power, scientists and engineers have developed the fourth generation of nuclear power plants.

The fourth-generation nuclear power or Generation IV reactors are planned commercial based reactor technologies being developed by the Generation IV International Forum (GIF). This international consortium endorses its members in active collaboration to overcome the current weaknesses within the nuclear power industry and develop advanced nuclear systems that can meet the world's future energy needs. With the objective to have the nuclear energy systems deployable no later than 2030, four broad areas were identified by GIF to set out technology goals significant to realize the R&D efforts [1].

- SUSTAINABILITY: The nuclear energy systems must provide sustainable energy generation that meets clean air objectives, provide long-term availability of systems with effective fuel utilization and minimize the production of nuclear waste, reducing the long-term stewardship burden.
- ECONOMY: They must be advantageous over other energy sources in terms of lifecycle cost, and they must have a level of financial risk comparable to other energy projects.
- SAFETY and RELIABILITY: They should excel in safety and reliability in operations, have a very low likelihood and degree of reactor core damage, and eliminate the need for off-site emergency response.
- PROLIFERATION RESISTANCE and PHYSICAL PROTECTION: they must increase the assurance to become unattractive for diversion or theft of weapons-usable materials, and they must increase the physical protection against acts of terrorism.

The goals mentioned above are not easily quantifiable and are open to interpretation; for example, the economic goal, without a doubt, any small gas plant would constitute a financial risk smaller than any concievable nuclear reactor project. Nevertheless, based on these objectives, a lot of nuclear reactor proposals were assessed by GIF, and the experts identified the

six most promising reactor systems that could be further developed to meet the goals, as :

1. Gas-Cooled fast reactor systems (GFR)
2. Lead-cooled fast reactors systems (LFR)
3. Molten salt reactor systems (MSR)
4. Sodium-cooled fast reactor systems (SFR)
5. Supercritical-water-cooled reactor systems (SCWR)
6. Very-high-temperature reactor systems (VHTR)

Sweden has been conducting its R&D on Gen-IV nuclear technology for some time now, focusing mostly on lead-cooled fast reactors (LFR) with its particular expertise at KTH in the SEALER [2] reactor concept. In addition, the SUNRISE (Sustainable nuclear research in Sweden) project takes the initiative in constructing a lead-cooled research reactor to battle the climate crisis for the future society. The reactor will provide irradiation services of fuels and materials for Gen-IV reactors and advanced modular reactors and develop safety assessment strategies for a potential global deployment of Gen-IV lead fast reactors.

The lead-cooled fast reactors are nuclear reactors that feature a passively safe design operating at a fast neutron spectrum with high temperatures and near atmospheric pressure conditions. The fuels anticipated for this reactor scheme are either metal oxide or metal nitride cooled by molten lead (or lead-based alloys). The concept, in general, is similar to that of the SFR; the choice of the coolant is the feature that entails a long list of advantages[3]:

- As a dense liquid, lead has nuclear properties like low neutron absorption, enabling a fast reactor to maintain a hard neutron energy spectrum, resulting in a longer core life and improved resource utilization.
- The coolant has a very high boiling point (1737°C), making it compatible with high-temperature operations and does not require strong pressurization, thereby reducing the risk of loss of coolant accident.
- Lead is a relatively inert liquid coolant that does not react with water or air, unlike sodium that can explode when in contact with water or burn in air. This chemical inertness eliminates the need for an intermediate coolant circuit, allowing an increased efficiency over SFRs.
- Lead has a high thermal capacity and high latent heat that allow significant thermal inertia in the event of loss of heat sink.
- The low coolant moderation allows a flexible core design with greater spacing between the fuel pin lattice, reducing the core pressure losses; This, coupled with the thermal

properties of lead, allows a high level of natural circulation for cooling, making it possible to rely upon passive shutdown heat removal.

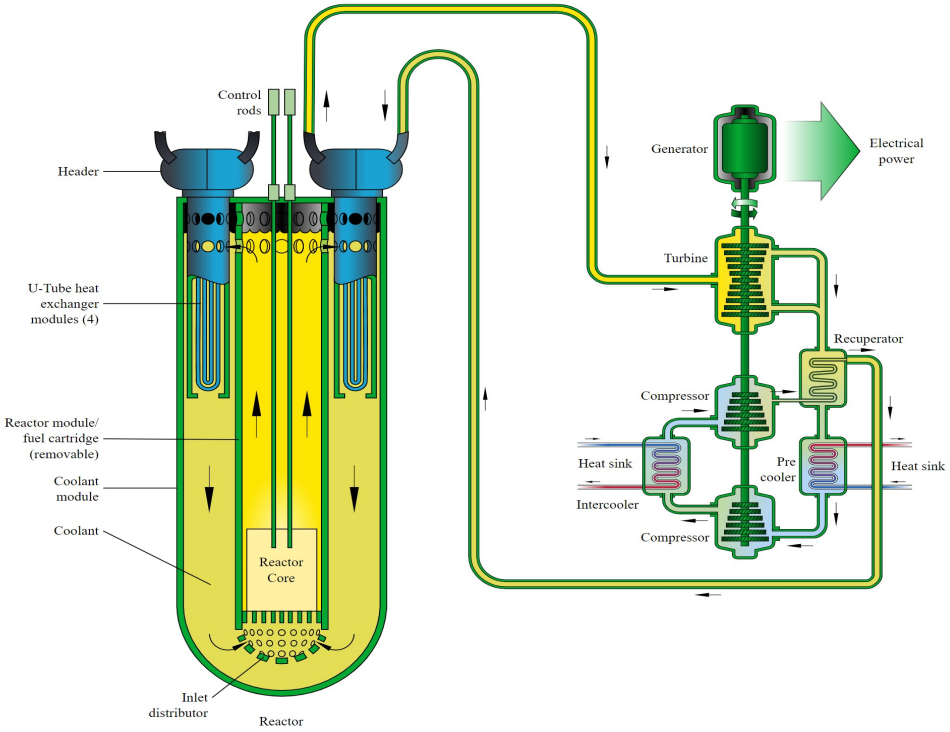


Figure 1: Graphical representation of a generation IV lead fast reactor.[1]

The thesis will be focusing on the nuclear fuel development of the SUNRISE project. The development of these fuels is here done using computer simulations. Fuel performance simulations are essential to reactor research as they provide computational solutions and responses to various uncertainties one might have towards the limitations of components. Understanding the fuel behaviour under operation is crucial from safety and performance standpoints, especially when a new fuel type is being explored. The simulations reduce the need for actual irradiations in a reactor by providing quick, relatively cheap, and precise answers to questions that may arise in the multidisciplinary subject of safety that may be social and technical.

2 LITERATURE REVIEW

2.1 Fuel Performance

2.1.1 Fuel Performance Overview

From a safety and performance perspective, whenever a new fuel is being developed, it is crucial to know the general behaviour of the fuel during its entire lifetime from production to storage. It is ideally essential for the nuclear fuel to effectively release its fission heat during operating conditions while retaining all of the fission products. However, many physical phenomena occur in the fuel pellet. The fuel material that is continuously evolving due to irradiations starts experiencing mechanical stresses due to the differential dilatations created by the temperature gradients. These mechanical stresses deform the pellets. Simultaneously, the porosity changes and defects from the initial structure travel to the grain boundaries inducing densification. The densification is then overcome by swelling, which is induced by the build-up of fission products. Fission products (e.g. Kr and Xe) diffuse in the matrix and form bubbles. This induces creep through irradiations and swelling of the fuel rod reduces the fuel-clad gap. Many other phenomena occur in the fuel as the burn-up increases, such as the release of fission gas or cracking. Hence analysis needs to be thoroughly done to depict the fuel behaviour pertaining to safe reactor operation.

It is essential to understand that nuclear fuel is constantly transforming during its life (production-operation-storage). Most of the present understanding that involves modelling fuel deformation mechanisms remains empirical and cannot easily be extrapolated to new fuel compositions environments or operating conditions. Moreover, analysis can be performed by directly interacting with the fuel during its production and storage phases in its lifetime. Since existing commercial reactors today are not typically built for several shutdowns or experimental purposes, the fuel analysis during the operation phase becomes more complex, especially when civil work is involved, the cost goes up. Reactors have to be then explicitly designed for experimental purposes in order to interact with the fuel.

Previously experimental reactors performed analysis on fuels and materials using an Edisonian approach of trial and error. The repeated experimental testing and irradiations were time-consuming and highly expensive. Today, with the help of computational tools, some of these tests can be simulated. Fuel designers, research institutes, safety authorities, and a nuclear power plant's utility use simulation tools for various purposes like design optimization, safety analysis, to aid and guide experimental research. Such tools that help us simulate nuclear fuel

behaviour can be categorized as fuel performance codes (FPC). FPCs may be designed to model the thermo-mechanical state of the nuclear fuel (intended as fuel and cladding) that has feedback on the neutronic and thermo-hydraulic behaviour of the physical state of the core. It simulates the fuel behaviour at the scale of a fuel rod or fuel assembly. The simulation of a fuel rod considers several phenomena occurring in the nuclear fuel (e.g. the fuel thermal conductivity, the mechanical interaction between the fuel rod components, fission product release, creep, cracking, swelling). For safety analysis, the models of the above parameters are fitted against experimental data to ascertain that no fuel melting could occur. Such dedicated computer codes model the nuclear fuel performance.

2.1.2 Modelling of Fuel Performance

The modelling of the fuel behaviour is a multifaceted task as many of the phenomena described above interact with each other in complex manners and take place at different time and length scales. Opting for a multi-scaled modelling approach enables the computation code to couple the models of various phenomena across the different scales for e.g atomic, microscopic or macroscopic scale within the FPC. However, this project will be looking into the aspects of the fuel from a macroscopic perspective following what is already present in the FPC. Here the fuel encounters severe thermo-mechanical environments and its responses are usually in the form of creep, swelling, cracking or pellet-cladding interactions. These macroscopic responses are usually influenced by a heterogeneous microstructure that is interdependent on temperature gradients and burn-up. Hence the use of a multi-physics and multi-scale approach to elucidate the behaviour of fuel in such complex environments is needed.[4].

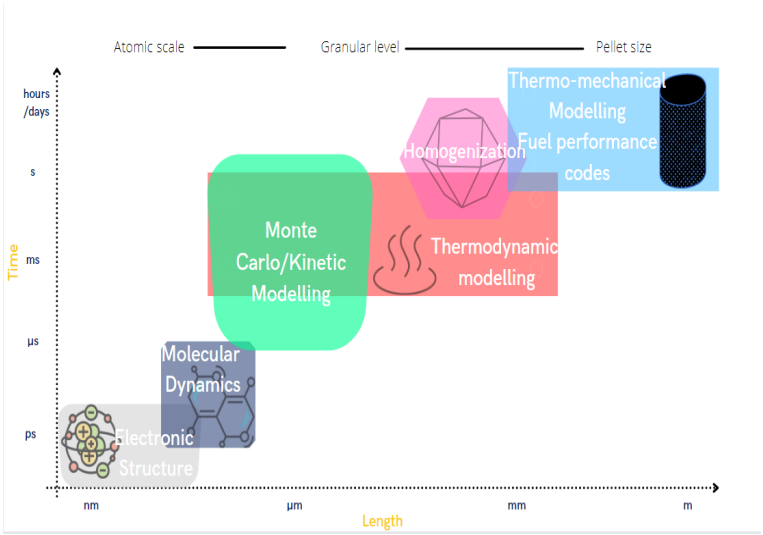


Figure 2: Adapted representation of the scale spanning the modelling of nuclear fuel from atoms to the pellet.[4]

As the title suggests, the thesis will be exploiting a FPC written in a Fortran environment developed by JRC (Karlsruhe) called TRANSURANUS [5]. TRANSURANUS (TU) is a tool capable of simulating the fuel behaviour under a nuclear reactor's normal operating and accidental conditions. Predicting in-reactor fuel performance requires introducing assumptions right from the start to obtain a sufficiently accurate numerical solution. The TU code represents the cylindrical fuel rod in a quasi-two-dimensional or 1.5D way. All transport processes are solved in one dimension, typically radial, and the axial segments are coupled via balance equations. Hence, the solution of the transport processes is usually programmed in separate modules for each axial slice, using couplers to manage interactions between models and slices [6]. The code also includes a wide-ranging material data bank for oxide, mixed oxide, carbide, and nitride fuels, along with cladding and coolant options. Finally, there is an availability of choices between using statistical or deterministic solvers. The TU code is a well-defined mechanical-mathematical framework incorporating physical models to obtain fast and reliable results. A discussion on how the TU code has been implemented is mentioned in the later sections.

2.1.3 Fuel Performance Parameters

There is a possibility of using two types of fuel in SUNRISE LFR, namely UO_2 and UN. Hence, for this project, the focus in the simulation is with respect to these two fuel types. UO_2 is a fuel that has been globally accepted today in almost all kinds of reactors. Through immense irradiations over decades of work, the data obtained for this fuel type has verified models that accurately exemplify the fuel behaviour. Thus, giving us standardised values required as inputs if one has to verify the responses concerning many phenomena of fuel behaviour analysis. However, the same is not true for newer fuels like UN. Although UN was a fuel developed initially for space reactor programs [7], there is very little data available. Also, the irradiation data available on the database on the models of the fuel behaviour can vary.

From the literature review, it is clear that the main property of concern with respect to fuel performance is fission gas behaviour[8][9]. Although some existing models depict the fission gas behaviour in UN, the present thesis adopts the available models following what is recommended in TRANSURANUS. The objective here is to analyse the fuel pin performance, a complex process involving the integration of a wide range of phenomena. Hence, it is crucial to correctly understand the fission gas behaviour from a safety point of view regarding failure criteria[10]. It consists of many processes: fission gas generation, diffusion, retention, and release. Each of them is detrimental to fuel performance [11].

- To start with the generation of fission gas, one could mention that the irradiation of fuel with time leads to the inevitable production of fission gases. These fission gas atoms created can cause crystallographic defects in the fuel as they possess high kinetic energy.
- Subsequently, when the temperature is sufficiently high, these gas atoms can diffuse in the fuel lattice and form bubbles. The precipitated bubbles filled with low conductivity gas reduces the fuel's thermal conductivity, thereby leading to higher fuel temperatures similar to that of a denser fuel. Increased temperature is vital from the fission gas release point of view as it promotes the migration of atoms frozen in the pellet matrix and releases the gases close to the grain boundary.
- Whereas for the fission gases retained in the fuel, a nucleation process begins around the fuel's grain boundary, which increases the volumetric swelling of the fuel pellet. The swelling adversely increases the risk of pellet-clad mechanical interaction to cause the failure of cladding.
- To conclude, If the gas is released from the fuel, the pressure within the fuel pin increases, subjecting the cladding to severe stress. The extent of gas released is important from a safety perspective. It can be a potential hazard (biological) in case of an accidental cladding rupture during operation or transportation of spent fuel.

The fission gas behaviour itself has several complex concomitant parameters/phenomena that need to be considered while performing analysis. To summarise, the changes in fuel density (caused by swelling and densification) affect the pellet-cladding gap, thereby affecting the gap conductance and fuel temperature. In addition, the fuel swelling induces axial strain to the cladding resulting in elongation changes. This study will examine how different kinds of models impact some of these operational parameters that are significant to fuel performance

2.2 Sensitivity Analysis

Based on the fuel performance perspective, it can be postulated that nuclear fuel undergoes a complex deformation process. The underlying cause of this requires us to inspect the parameters and properties of the fuel that directly impact different phenomena that can occur during the lifetime of the fuel material. It is essential to understand that the various phenomena occurring in the fuel pellet are hypothesized by numerous existing models that depict the fuel behaviour pertaining to the phenomena. Thus, a sensitivity study would tell us which parameter or property of the fuel directly impacts the phenomenon occurring in the fuel based on the model used for the study.

For design applications, a sensitivity parameter study method is useful for ranking which of the design parameters have the most influence on the response quantities. A multidimensional parameter study is performed in this thesis, a technique that involves partitioning the domain of parameters and evaluating the objective function at those points. The results from the parameter study would help in a future optimization process to identify the system of inputs that are responsible for the overall uncertainties of the system, and to remove design parameters that have little or no influence on the responses.

To conduct the sensitivity and uncertainty analysis for the sunrise reactor study, a software framework developed at Sandia National Laboratories named DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) is used[12]. Although many software products are available that can perform sensitivity analysis[13], Dakota was selected since it is open-source and quite popular; The Dakota toolkit delivers a variety of iterative methods and meta-algorithms by automating a series of simulations where input quantities are varied to determine its effects on the simulation results. In addition, it provides restarting capabilities and the ability to capture simulation failure. It also exploits parallel computing and nested modelling [12]; One of the salient features of Dakota is its ability to flexibly interface it with almost any simulation code. For example, the Dakota toolkit can be coupled/interfaced with the fuel performance code TU. Thus, allowing for a broad range of iterative capabilities. This will be discussed in detail in the later sections.

A brief summary of the software's mathematical capability in terms of different algorithm classes supported is given below.

- Parameter Studies - Uses deterministic methods to identify the effect of parametric changes within a simulated model. This helps to explore key model characteristics/trends, robustness and non linearity that influences the choice of follow on UQ or optimization.

for e.g. Multi dim parameter study.

- Design of Experiments - Similar to parameter studies, but used to explore good coverage of the parameter space with minimal simulations in a design problem. for e.g. a global sensitivity analysis can be performed using a Latin hypercube sampling method.
- Uncertainty Quantification - uses a probabilistic approach to assess effect of input parameter uncertainty on the simulation model outputs. This helps the user to determine mean or median performance of a system and to find the probability of reaching failure/success criteria. for e.g. Monte Carlo sampling.
- Optimization - is a goal-oriented method that attempts to find the best performing design, scenario, or model agreement with respect to the parameters and responses. It helps to identify system designs with maximal performance and minimize cost over system designs/operational settings by determining best/worst case scenarios. for e.g. Pareto-set optimization
- Calibration - an algorithm that determines the parameter values that maximize agreement between simulations and experiments. For E.g. Bayesian calibration.

2.3 Accelerating Fuel Development

A sensitivity study is important to assess the capabilities of a FPC accurately. It demonstrates the robustness of calculations and helps to characterize the possible reasons for discrepancies between trends or values observed in the calculations. Hence, the user can improve on the code/design of fuel based on optimization. Furthermore, justifying uncertainties and calibrating the code gives a premise for bench-marking the fuel to qualify for validation purposes by a regulator. Fuel manufacturers would want to follow a similar pattern when developing any new type of fuel, as suggested by Terrani et al [14]. The paper suggests the entire nuclear community could implement separate effects testing to accelerate fuel development. The outlined approach suggests to devise a three-phase programme that would accelerate the fuel development, where phase 1 is an emphasis on the thermodynamic and neutronics assessment of the fuel system to rapidly identify the compatibility between its constituents and its ability to withstand the irradiation environment based on the application. Phase 2 is an iterative exercise of engineering-scale modelling and simulation tools, combined with separate-effects testing. The approach of this method is to subject the fuel materials to a broad range of operational parameters. Once the governing properties of the fuel impacting parameters and phenomena are identified, they are then ranked in order of priority. The parameters that belong to the high impact and high uncertainty sector are prioritized for targeted separate-effects testing. This iterative process of

separate effects testing is used for subsequent model development/refinement to ultimately meet the required criteria of standardized specifications by a regulatory body. Figure 3 illustrates the iterative flow of the activities involved in this phase.

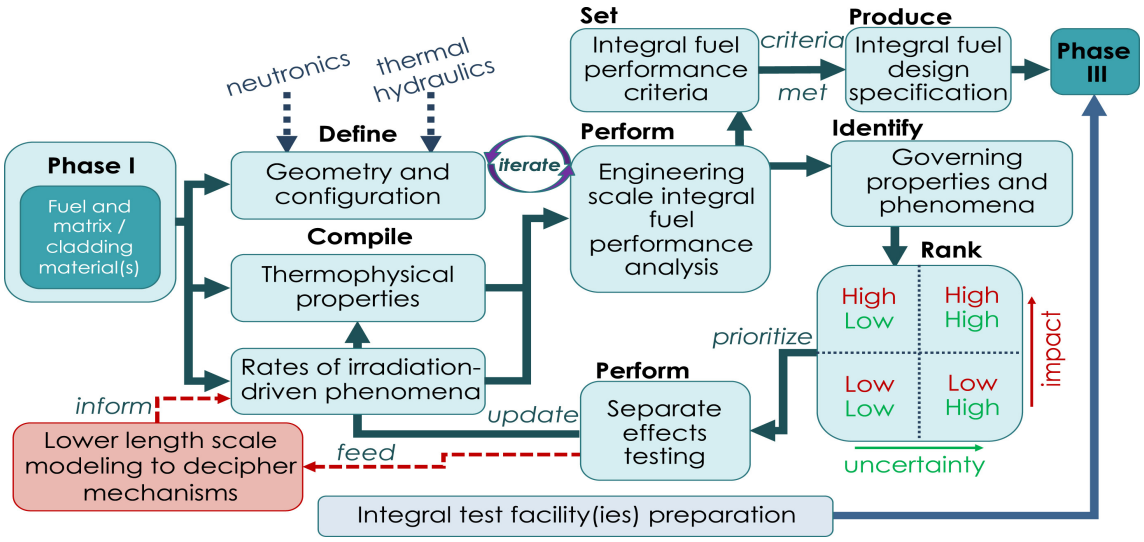


Figure 3: Iterative flow representing the separated effects testing.[14]

The final phase of this approach is to make use of a testing facility/experimental reactor to validate the safety and performance of the fuel system through targeted integral irradiation tests. Phase 2 lays out the foundation for the safety case that models all of the fundamental phenomena pertaining to the fuel behaviour, the purpose of performing experimental transient testing at different burn up levels is to ensure that all important phenomena and their complex inter-relationships are fully accounted for and that there is no unexpected performance to deter the licensing process. This phase ensures that after successful trials, modifications in the manufacturing source can be implemented to support the goal of the end user without impacting the licensing basis, as long as the fuel design specification and primary material configuration, composition, and microstructure is standardised.

3 SOFTWARE IMPLEMENTATION

This section will focus on how various softwares can be implemented to obtain the relevant data through modelling and simulation. A Linux based system was built that encompassed the libraries to compile TU and the Dakota software toolkit, and a script was made in order to couple the softwares. Finally, a python package is used to plot the results in a ranked form. The following parts of this section address how the work was performed.

- TRANSURANUS: Uses an input file that allows the user to simulate the fuel rod's behaviour, thereby generating an output file containing several simulation results.
- Dakota: Requires an input file that contains the model input parameters of TU that can be used for user-specific purposes, like multidimensional parameter study. The output is a data matrix.
- Bash script: This script couples the two software together by converting the input defined in Dakota to run TU. it grabs the output obtained from TU and sends it to Dakota.
- Python package: This package allows us to read the large matrix output obtained from Dakota and identify the relevant correlations in the parameters based on desired results.

3.1 TRANSURANUS

As mentioned earlier the TU code is used to simulate the mechanical, thermal and physical behaviour of fuel rods based on the SUNRISE reactor conditions. The code was specifically designed to analyse a whole rod in a 1.5D cylindrical geometry by adopting axisymmetry. The axial discretisation of the fuel rod consists of a stack of cylindrical fuel pellets (either UN or UO_2) and 15-15Ti cladding separated by a helium-filled gap, as shown in Figure 4. Each slice is analysed at the middle, and all the time dependant input quantities are constant along the slice (e.g., linear heat rating). Being a comprehensive data bank for materials, it also contains most of the present-day physical models of the fuel in terms of densification, swelling, generation of fission gases, and several other models that allow the code to deal with a wide range of different situations.

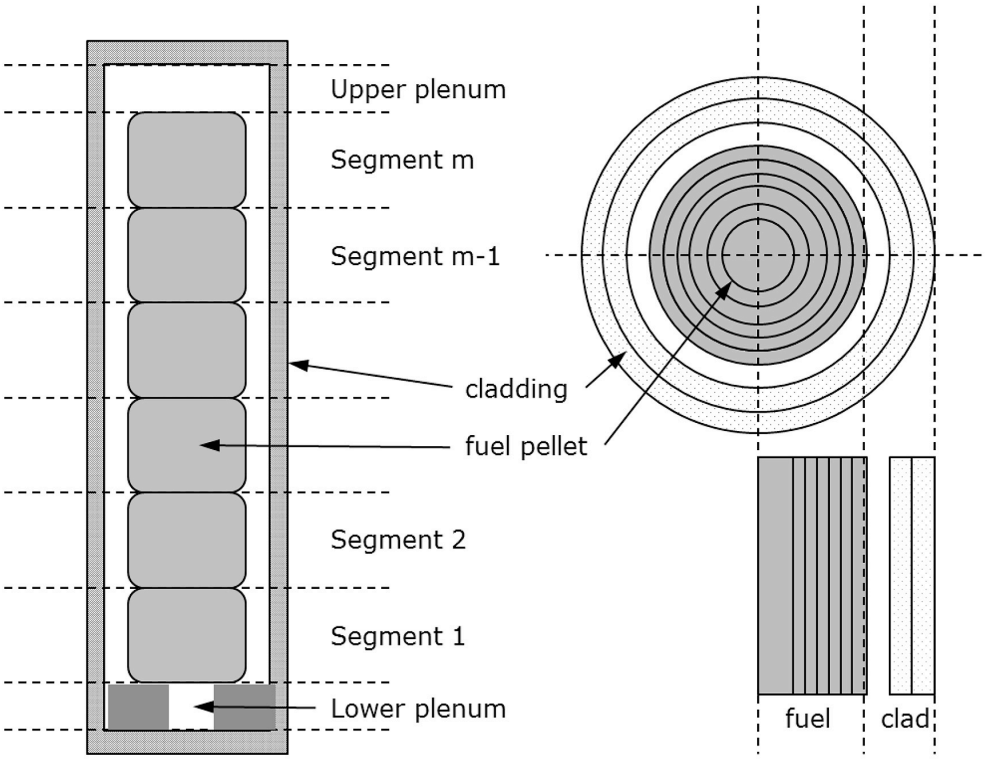


Figure 4: Discretisation of fuel rod.[6]

3.1.1 Input-Setup

The TRANSURANUS FPC is used as a BlackBox. In order to execute a simulation, the code requires an input file with complete data. The data present inside the input file determines the type of reactor, the fuel and its geometry, the coolant, heat transfer coefficients, the rod power and time of computation. This data in the input file can be categorised into three types. The first group represents the *control options*; that allows the user to select between the different models that describe the interacting phenomena affecting the fuel pin performance and material behaviour (e.g. selecting the model for FGR). The second group is the *fuel composition parameters*; these may be various geometrical and physical quantities that must be input by the user (e.g. radius of cladding). The third group represents the *macro time step inputs*; some data vary as a function of time (e.g. linear rod power, coolant temperature). The user must select a set of time steps and set the values of these quantities at each time step.

As a general setup for calculation purposes, the active length of the fuel rod is divided into 10 axial segments or slices in the code. The analysis is performed from slice 1 to slice 10. In addition to these slices, an extra slice is also modelled to account for the upper gas plenum. For the radial discretization, the fuel and the cladding are partitioned into 6 coarse zones, Five for the fuel and one for the cladding.

Some boundary conditions implemented to the code are :

- The linear rod power is considered maximum at slices 5 & 6 .
- The inlet coolant temperature is considered for the time dependent coolant temperature. (IWERT = 9)
- Monte Carlo statistical analysis is not opted for hence the analysis is deterministic. (istati=0)

Once a user has all the required information set for the input file, the analysis can be performed. In this thesis, predefined information relating to the neutronics data for the reactor was used as input for the TU code. Furthermore, The 5^{th} slice is taken into account for all calculation purposes used in chapter 4.

Table 1: Relevant TRANSURANUS input parameters

Fuel characteristics	
Fuel type	UN or UO_2
Cladding material	15-15Ti
Fuel enrichment	11.9 %
Fuel porosity	5 %
O/M ratio	2.0
Fuel grain size	10 μm
Geometry	
Fuel pellet diameter	9.802 mm
Active fuel length	1060 mm
Gas plenum length	160 mm
Cladding inner diameter	10.202 mm
Cladding outer diameter	11.202 mm
Coolant flow rate	2.40E+06 g/h
Coolant temperature	420 °C
Coolant pressure	0.1 MPa
Linear rod power	11.91 kW/m
Fast neutron flux	4.11E+14 $cm^{-2}s^{-1}$

3.1.2 Output-overview

After the input file is prepared, and the calculation is performed correctly without any syntax error, the TU code generates an output file containing all the data associated with the fuel rod calculated for each specified time frame. Additionally, it provides data relevant to each slice or section of fuel, such as fuel centre temperature, gap conductance, burn up, fuel elongation, etc.

3.2 Dakota

Dakota provides an interface between the simulation code and the iterative analysis method. Dakota can be used to couple the simulation code in an iterative fashion to perform a Multi-Dimensional Parameter Study on the inputs. The output variables can be analysed by varying the basic parameters and material properties in the TU simulation code. The user provides the desired inputs within which variation of a property is to be analysed, and the randomized sets of data will be generated for the purpose through Dakota.

A study in Dakota is typically defined in an input text file (.in extension), which defines the user input variables, responses for the study, and the type of analysis being performed. First, Dakota writes a parameter file containing the current variables used to create the input file for the TU simulation execution for each iteration. Then, the simulation process is executed as an external process using a bash script. When the simulation finishes, it reads the responses from the simulation's output file, stores them into the Dakota results file, and runs its internal iterator to provide new variable input for the next program call. This procedure is repeated until the complete iteration of the study is finished. After the iteration study is completed, the responses and variables are written to an output file (.out extension), usually of tabular data or HDF5 format. Since Dakota only uses the parameter values and objective functions and has no need to know the internal functionality of the simulation code, it can be inferred that its operational as a Black-Box optimizer. The samples that are generated through this are then investigated upon by making use of correlation coefficients. A graphical representation of an iterative Dakota process is shown in Figure 5. The dashed lines in the figure indicate the transfer or conversion of data managed by a script file defined by the user since these processes depend on the traits of the simulation code. The solid lines in the figure represent the processes built-in into Dakota or the simulation code.

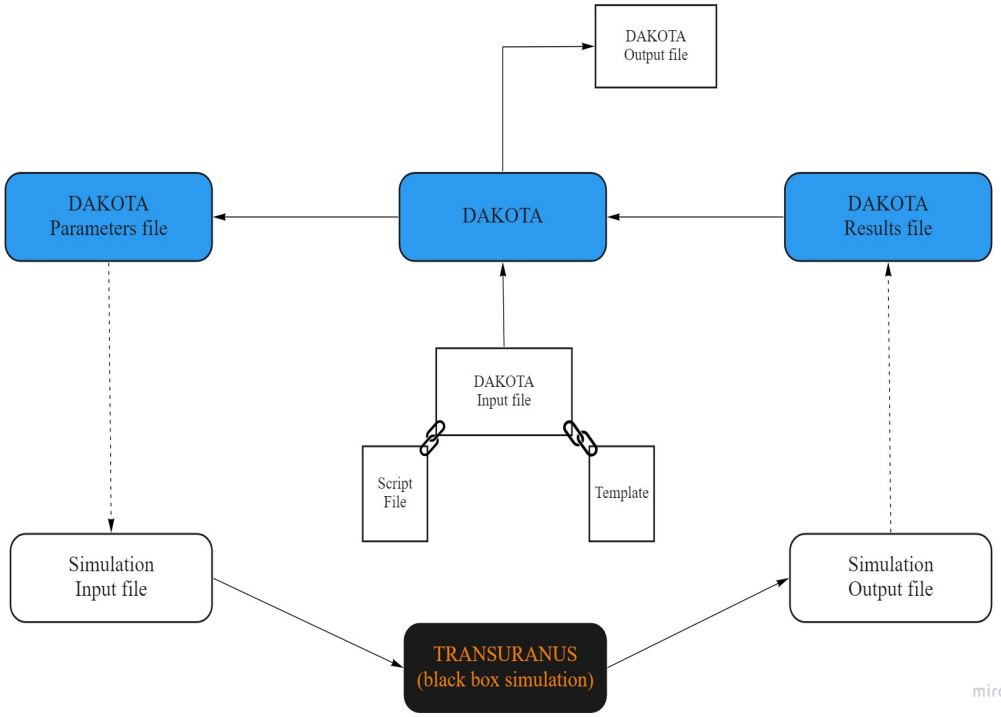


Figure 5: A schematic diagram of the Dakota iterative process with the ”black box”. [12]

3.2.1 Input-Setup

Dakota uses only a single file that contains all the information required to run an analysis. Figure 6 shows an example of the input file containing several blocks that tell Dakota what to do. The blocks are :

- Environment: This keyword block specifies general global Dakota settings, such as configuring which output files Dakota will generate after running. In the example (Figure 6), the environment block is configured to generate a tabular data file containing variable and response data. The environment block is optional, and a maximum of one environment block can appear in a Dakota input file.
- Method: This block in the input file specifies which iterative method Dakota will employ and the associated options for that method. In the example (Figure 6), the keyword multidim_parameter_study calls for a multi-dimensional parameter study while the keyword partitions specify the number of intervals per variable. There are 2 intervals or 3 data points evaluated between the lower and upper bounds specified in the variables block. Another choice for the method section is sampling with LHS. Multiple method blocks can appear depending upon the type of study.

- Model: This block is optional in the Dakota input file that specifies the type of model that Dakota will use. A model provides the logical unit for determining how variables are mapped into a set of models.
- Variables: This block specifies the number type and characteristics of the parameters that Dakota will vary. Variables can either be continuous or discrete; they can be classified as design variables, uncertain variables or state variables. In the example, two uniform uncertain variables are present. The sub specification for the variables provides the descriptors 'r' & 'beta', as well as the lower and upper bounds for these variables. The information about the variables is provided in column format for readability. At least one variables block is required for a Dakota study.
- Interface: This block of the input file specifies the simulation code that will be used to map variables into responses as well as details on how Dakota will pass data to and from that code. In the case of this thesis, the interface block is defined in a way to communicate with TU. In order to run an external simulation like TU the command 'fork' is used, this command is a recommended option by the Dakota manual and a Linux operating system uses the fork function family to manage the simulation drivers and codes[15]. The analysis driver defines the test function that is being called upon, in this case the driver.sh is used as the coupling script. More detailed information on the coupling script is provided in Section 3.2.2. At least one Interface block is required for a Dakota study.
- Responses: This block specifies the types of data that the interface will return to Dakota from the analysis code TU. This block can include additional information such as constraints and derivative information. Since there are no constraints or derivatives associated with the parameter study, the keywords no_gradients and no_hessians indicate that no data will be provided by the method. At least one responses block is required for a Dakota study.

```
environment
  tabular_data

method

 multidim_parameter_study
  partitions 2

variables

  uniform_uncertain 2
  descriptors 'r'  'Beta'
  lower_bounds 4.40  0.2
  upper_bounds 4.60  0.33


responses

  response_functions 10
  descriptors 'FCT1' 'FCT2' 'FCT3' 'FCT4' 'FCT5' 'FCT6' 'FCT7'
  'FCT8' 'FCT9' 'FCT10''
  no_gradients
  no_hessians


interface


  link_files 'template' 'driver.sh'

  work_directory named 'workdir/run'
  directory_tag

  parameters_file 'params.in'
  results_file 'params.out'

  file_save
  directory_save

  fork
  analysis_driver 'driver.sh'

  #Parallelization on the local CPU
  #asynchronous
```

Figure 6: An example of Dakota input text file

3.2.2 Bash- Coupling script

As mentioned earlier, Dakota is an interface that allows to us to run multiple TRANSURANUS calculations for a sensitivity study. In view of this, a script file and a TU input template file was prepared. The coupling allows Dakota to read & convert the input, Run TU and then collect the output. Before running a bash script with Dakota, a template file is required, which is very similar to the input file of TU but has the desired parameters required for the study within braces { }. The bash script file (.sh extension) is made with a set of commands invoked to perform the following operations in the particular order as mentioned below.

1. It first Collects the parameters generated by Dakota.
2. It invokes the preprocessor built-in Dakota ‘dprepro’ which creates an input file made for the simulation code using the collected parameters from Dakota.

3. By making use of the input file created by dprepro, the TU executable is run.
4. After the execution of TU is completed the post processor is called to extract the responses quantities of interest and write them into the results file.

3.3 Output Processing- Python

Python packages such as numpy, pandas, seaborn, matplotlib and h5py were used to perform the output processing. They are employed because they have good capabilities of handling data and creating graphical representation of the results. For example to calculate a Spearman correlation coefficient[16] for the variables and responses obtained from the Dakota study, a jupyter notebook file was created containing these python packages that allowed us to run the correlation analysis.

The Spearman correlation coefficients are a measure of the possible correlation existing between two parameters. The coefficient can vary between -1 and +1, 0 implying no correlation and considered significant only when the absolute value exceeds 0.5. The larger the absolute value is, the stronger the correlation is. The positive sign implying the value is directly proportional where as a negative sign indicates an inverse relation.

4 FUEL PERFORMANCE ANALYSIS

This section presents the main TRANSURANUS simulation results of the SUNRISE LFR irradiation (normal operating) conditions. Analysing the behaviour of the irradiated fuel pin in the most accurate way requires a comprehensive selection of physical models and correlations. Since TRANSURANUS offers a wide range of options that describe the same phenomenon or material property, the first task is to identify all the alternatives suitable for the simulation. In this context, a reference case was set up comprising all the model options recommended by the TU manual. This indication is based on the model options that are most reliable or widely assessed. Although some options suitable for precise ranges and conditions are available, the physical models primarily addressed to FBR conditions are selected. The material property choices are displayed in Table 2. In Table 3, some of the relevant input physical model choices and modelling options of the reference case are listed.

Table 2: Material property input choices

	Material correlation	Input file
Fuel option 1	MOX fuels for FBRs - according to Többe/IAMBUS for UO_2 [17]	`MPgen_fuel=03`
Fuel option 2	Uranium Nitride	`MPgen_fuel=16`
Cladding	1.4970 austenitic stainless steel annealed and cold-worked according to Többe [17] applicable to 15-15Ti	`MPgen_clad=2`
Coolant	Lead - liquid state	`MPgen_cool=6`

Table 3: Physical model choices and modelling options selected in reference case

Phenomenon	Adopted model	Input file
Behaviour related physical models		
Fission gas release	URGAS algorithm [18] with diffusion coefficients of H. Matzke [19]	`FGDiff=6`
Diffusion equation for calculating the intragranular FGR	Diffusion equation is solved by the FORMAS algorithm with six exponential terms [20]	`iDifSolv=6`
Intergranular FGR	Simple grain boundary fission gas behaviour model [20]	`igrbdm=1`
Densification	Simple empirical densification model [20]	`idensi=2`
Relocation	Modified FRAPCON-3 model [21] [20]	`ireloc=8`
Grain growth	Model by Ainscough [22] and Olsen [23] reviewed by Botazzoli [24]	`igrnsz=1`
Gap thermal conductivity	URGAP model [25] thermal conductivity of mixture by Lindsay and Bromley [26] with accommodation coefficients	`ihgap=0`
Other modelling options		
Central void formation	Manufacturing geometry of fuel may change as a result of post-sintering, melting, creep, etc	`izenka=1`
Internal rod pressure	The inner pin pressure is calculated as a function of temperature and moles of filled gas and fission gas released	`ivar=2`
Fuel rod analysis	At the beginning of the calculation the fuel rod and cladding are not in contact	`ifall=3`
Power density form factor	Assumes that the local power density is proportional to the neutron flux	`iform=0`
Geometry of the coolant channel	Hexagonal configuration	`ikueka=1`
Coolant heat transfer coefficient	Calculated by TU [20]	`ialpha=0`

4.1 Comparative Study

This comparative study is performed to understand the general behaviour of both the fuels UO_2 and UN relevant to the SUNRISE LFR using identical operating conditions and the same geometry. This choice of identical operating conditions between UO_2 and UN is a simplification and not what is expected for the actual reactor, since the core for the UO_2 fuel has not been properly designed yet. Although both fuels have different material compositions and properties, the comparison is performed since the UO_2 correlations are very well-validated, having an extensive database available. Hence the model is more reliable and has some merit.

The fuels are subjected to the maximum possible reactor operational years, i.e., without any failure reported by the TU code (e.g., clad rupture). The outputs are extracted for each fuel separately.

4.1.1 Temperature Comparison:

Figure 7, displays the temperature profiles of both fuels. The interesting detail here is that the fuel centre temperature (FCT) for the UN fuel has a different trend than that of the UO_2 fuel. This is a quite natural difference we can expect since the UO_2 and UN fuel have completely different thermal conductivities. The FCT is an important identification factor to look at since it gives information about the thermal conductivity of the fuel, the gap width, and the gap conductance.

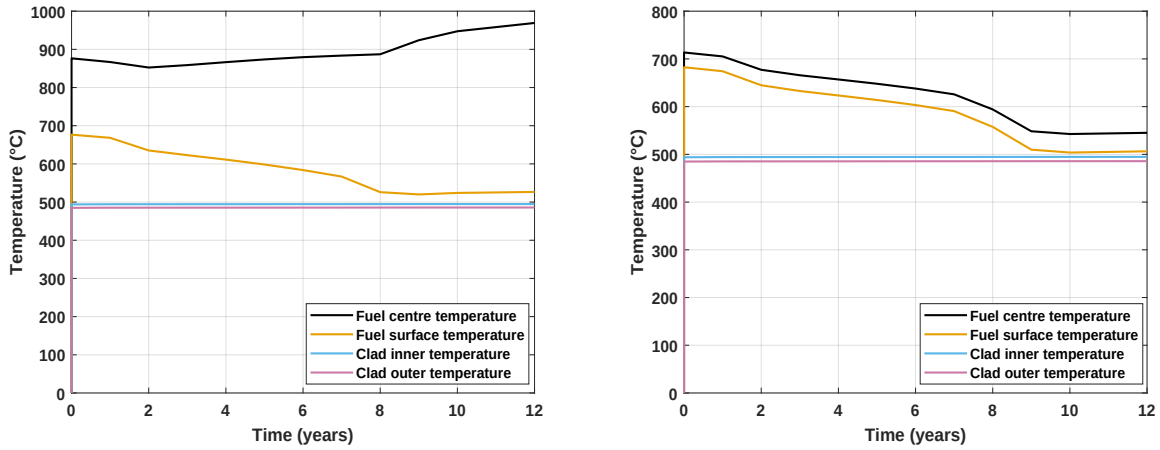
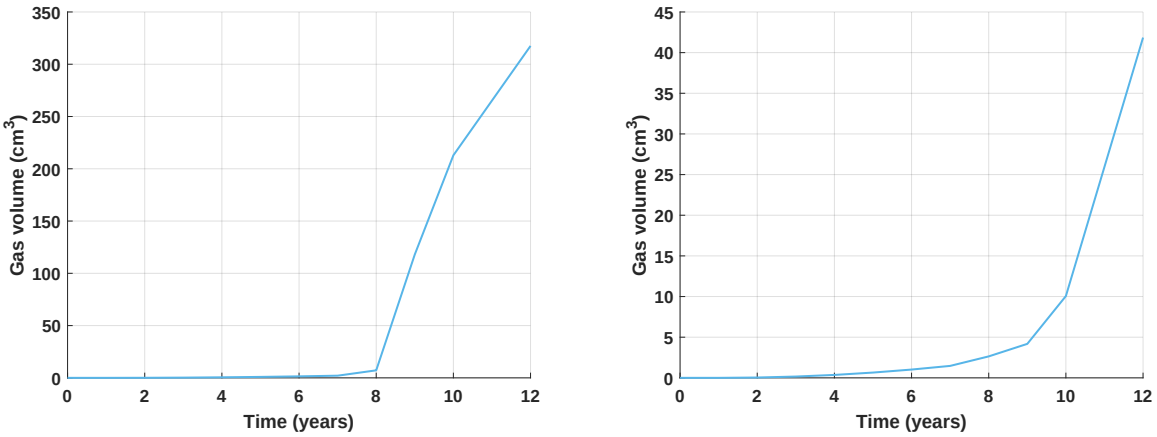


Figure 7: Temperature Profiles for (a) UO_2 and (b) UN.

4.1.2 Fission Gas Release:

From Figure 8, it can be observed that, the UN fuel releases lower amounts of fission gas than the oxide fuel. A combination of lower operating temperature and smaller temperature gradients in nitride fuels may explain this lower gas release [27]. Also at EOL, there is an exponential increase in FGR; this is because of the increased burnup with time. The most important parameter determining the FGR is the fuel structure. The gaseous fission products retained in the fuel may increase the fuel swelling and lead to further increase PCMI (Pellet Cladding Mechanical Interaction). Since the mechanism controlling this release appears to be atomic diffusion, the various isotopes of fission products such as xenon and krypton created inside the fuel grains tend to diffuse or precipitate into intra- and intergranular bubbles, ultimately leaving the fuel pellet.[28] The release of fission gas from the fuel pin into the upper free plenum may increase the inner pin pressure and thereby reduce the lifetime of the fuel rod, which is a peak concern for the reactor's safety.



(a) (b)

Figure 8: Fission gas release for (a) UO_2 (b) UN.

4.1.3 Stress-Strain Comparison

From Figure 9 and Figure 10, a pattern can be observed for both the fuels for the gap closure and pressure built up in the cladding. Although the fuel and cladding were not in contact initially, around 8 years of reactor operation, the gap closes, and there is a sharp rise in pressure around the same time. It can be inferred that as the gap size reduces, the contact pressure increases. This gap closure is vital from a PCMI point of view. This pressure that might build up over time may cause permanent cladding strain and lead to a possible breach/rupture that allows fission products to escape into the primary coolant.

Furthermore, the worst case of UN fuel could be 8 years for gap closure. The correlations predict a higher time for gap closure, maybe because the fuel has high thermal conductivity. However, there is uncertainty in this reference model if the fuel were to behave like UO_2. Nevertheless, the gap should undoubtedly be open for at least 8 years. Since the two fuels showed similar trends in the graphs, other stress-related comparisons such as irradiation strain, thermal strains, and cumulative damage index for the cladding are not reported.

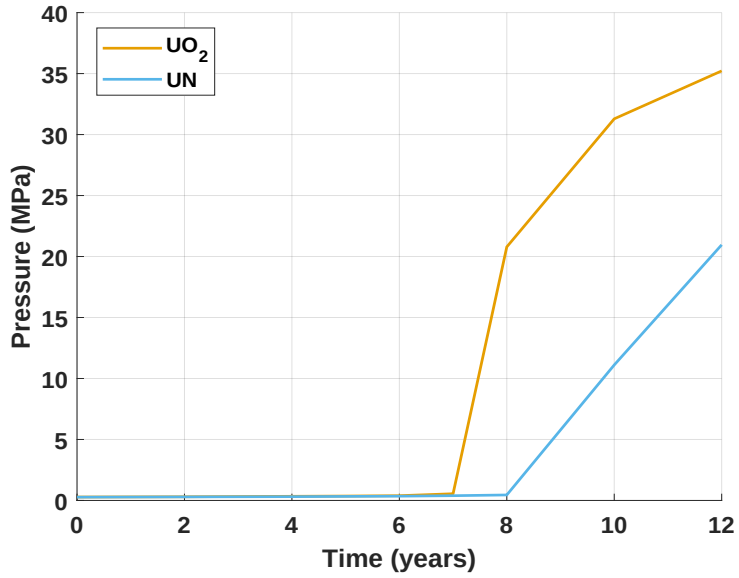


Figure 9: The inner cladding load for SUNRISE LFR reference case

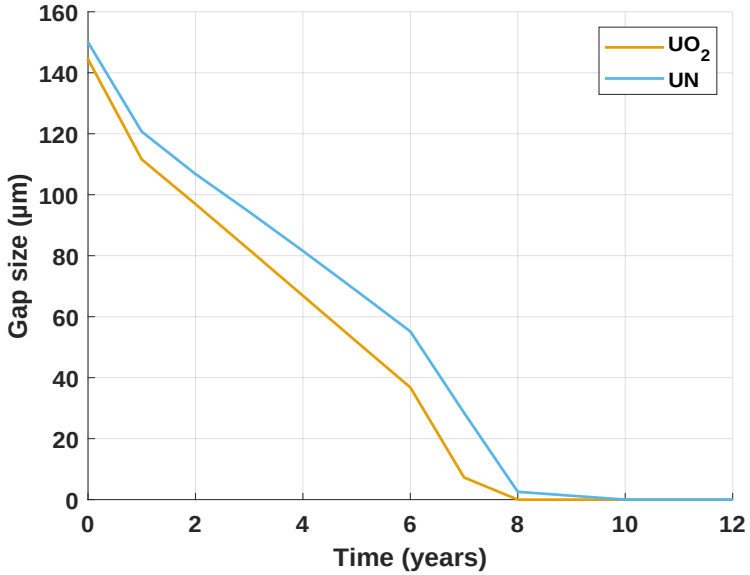
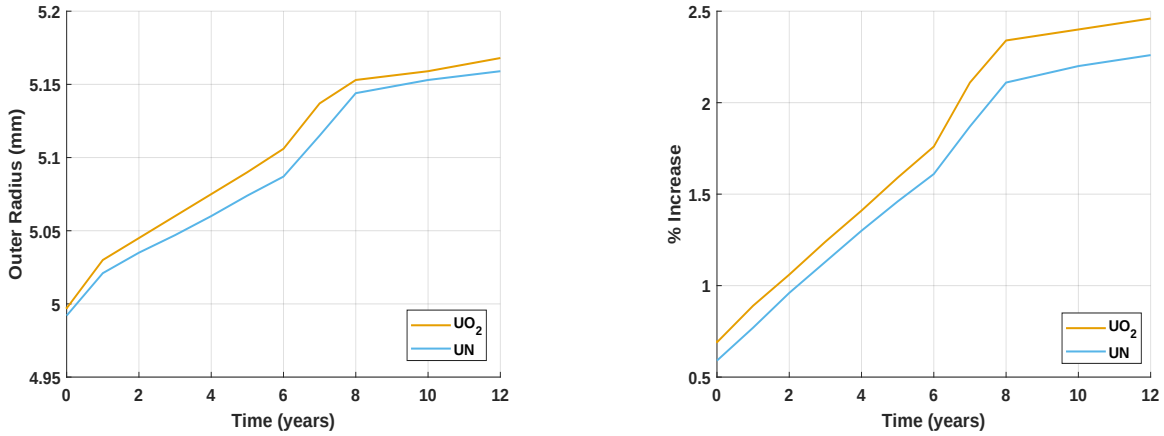


Figure 10: The gap size for SUNRISE LFR reference case

4.1.4 Geometrical Variation

In Figure 11, the geometrical variation in terms of fuel axial elongation and fuel outer radius for both fuels can be seen. Both fuels show a similar trend. Note that an initial fuel inner radius was not considered in the thesis, Although the option for the central void formation was used for the analysis, adopting the appropriate models for pore migration and densification. The TU code assumes that the central void can accommodate only a part of the fuel volume change; the other part contributes to fuel swelling[28]. The formation of the central void is unseen as the reactor operates at a reasonably low linear rod power and fast neutron fluence.



(a) (b)

Figure 11: Geometrical variation of both fuels in terms of (a) Fuel outer radius (b) Fuel axial elongation

4.2 Model Options

After the comparative study of both fuels from the previously performed stress analysis, it is well known that the gap dynamics are determined by fuel thermal conductivity and pellet deformation due to progressive fuel swelling. These models are essential as an error could influence almost all of the factors/parameters. Thus a suitable model is selected to conduct the sensitivity study. This part of the thesis will focus on just the novel fuel, i.e., UN, since the UO_2 already has standard verified models that have been experimentally tested and globally accepted. Therefore, the following actions are performed:

1. Check for various models within TU that describe the same phenomena for the reference case.
2. Conduct a sensitivity study focusing on these models and its parameters.

3. Select the best case scenario from the model options

The UN specific fuel properties implemented in the reference case are all denoted by model 15. The TU code automatically selects the model 15 option for all properties unless the user specifies a change in the input file. The table representing all the fuel specific model properties can be found in the APPENDIX. The Table 5 below represents the model options considered for the reference analysis and the sensitivity analyses

Table 5: Model options for the reference and the sensitivity analyses

Model	Options	Input file
Thermal Conductivity	Model according to Thetford et al.[29]	`ModFuel(6)=15`
	Model according to Hayes et al [30]	`ModFuel(6)=14`
Fuel Swelling	Model according to Coquerelle[31]	`ModFuel(4)=15`
	Model according to IAEA [32]	`ModFuel(4)=16`
	Model according to Ross [33]	`ModFuel(4)=49`

In the first action, there are two cases to be studied; Variation of fuel centre temperature based on the models for thermal conductivity and variation of fuel centre temperature based on the models for fuel swelling.

4.2.1 Thermal Conductivity Model

There are two Thermal Conductivity models available in the TU code with respect to UN. the simulation can be run for both models and the change in fuel centre temperature can be compared to pick the more accurate model. The LAMBDA coefficient in TU code depicts the thermal conductivity in the fuel, and the two models that are possible for selection in terms of UN are:

Model 14: Implemented by P. Van Uffelen as mentioned in Hayes et al[30], the experimental model data is valid for a correlation of UN with a maximum of 20% porosity within a temperature range of 298 K < T < 1928 K : and the correlation as :

$$\Lambda = 1.864 \times e^{-2.14P} \times (T)^{0.361} \tag{1}$$

Model 15: Thermal conductivity of Uranium, Plutonium nitride acc. to Thetford et al., J. Nucl. Mat. 320[29]. This correlation is only valid for temperatures below melting temperatures and

is given as:

$$\lambda_0 = \mathrm{AT}^2 + \mathrm{BT} + \mathrm{C} \quad \left[\frac{\mathrm{W}}{\mathrm{mK}}\right] \tag{2}$$

where

$A = 4.558 \times 10^{-5} y^3 - 7.734 \times 10^{-5} \mathrm{y}^2 + 4.180 \times 10^{-5} \mathrm{y} - 1.159 \times 10^{-5}$

$B = -1.044 \times 10^{-1} y^3 + 1.726 \times 10^{-1} y^2 - 9.464 \times 10^{-2} y + 3.307 \times 10^{-2}$

$C = 5.852 \times 10^{1} y^3 - 8.291 \times 10^{1} \mathrm{y}^2 + 3.051 \times 10^{1} \mathrm{y} + 1.326$

and

$\mathrm{y} = \mathrm{Pu/M}$

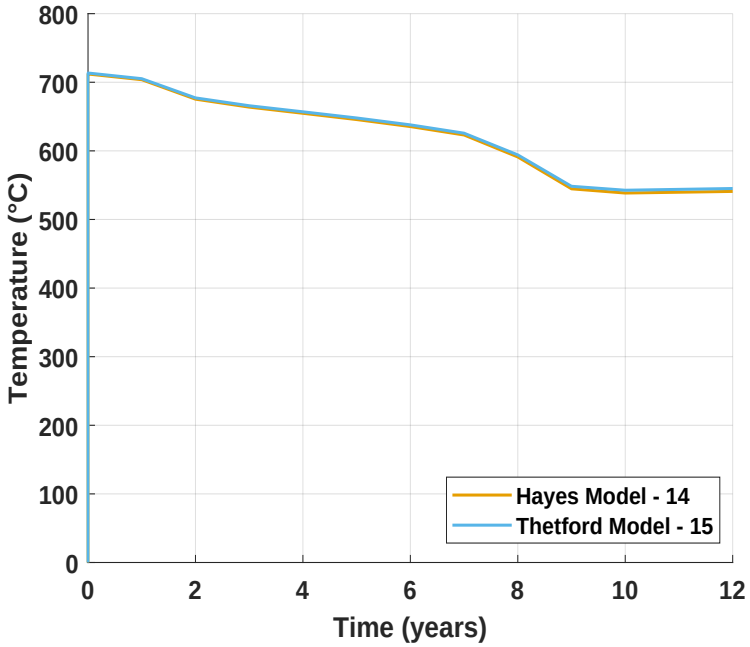


Figure 12: The variation of fuel centre temperature in lambda models

From the figure above both the correlation with respect to lambda have very less influence on the fuel centre temperature and hence it can be concluded that a change in thermal conductivity model is irrelevant for a sensitivity study.

4.2.2 Swelling Model

There are two swelling model options available in the TU code concerning UN. The Coquerelle model and IAEA model. In addition, a third model is scripted based on the already existing Ross correlation. The SWELOC coefficient in the TU code depicts the strain due to swelling in the fuel.

Model 15: The correlation proposed by Coquerelle[31] is expressed as a rate equation based on the increment of the fractional volume increase per burnup percentage. Given by the equation:

$$\Delta\frac{\Delta V}{V} = S\Delta bu \tag{3}$$

Where S is the swelling rate which is the increment of the fractional volume increase per burnup. S = 0.009 if the gap is open. The description is as mentioned in the TU handbook [20]

Model 16: This correlation is according to the IAEA TECDOC 1374[32], which gives the total swelling in volume fraction which takes into account the theoretical density of the fuel, burnup percentage and fuel central temperature according to the equation:

$$\frac{\Delta V}{V} = 1.16 \times 10^{-8} \times T^{2.36} \times bu^{0.82} \times D^{0.5} \tag{4}$$

Where T is the maximal central temperature , bu is the burn up percentage and D is the theoretical density of the fuel.

Model 49: This user-specific option setting in TU was scripted accordingly for the Ross correlation [33]. It suggests integral swelling as a function of fuel average temperature, given by the equation:

$$\frac{\Delta V}{V} = 4.7 \times 10^{-10} \times T^{3.12} \times bu^{0.83} \times \sqrt{\frac{\rho}{\rho_{td}}} \tag{5}$$

Where T is the average fuel temperature, bu is the fuel burnup given in atomic percent and ρ_{td} is the theoretical density of the fuel.

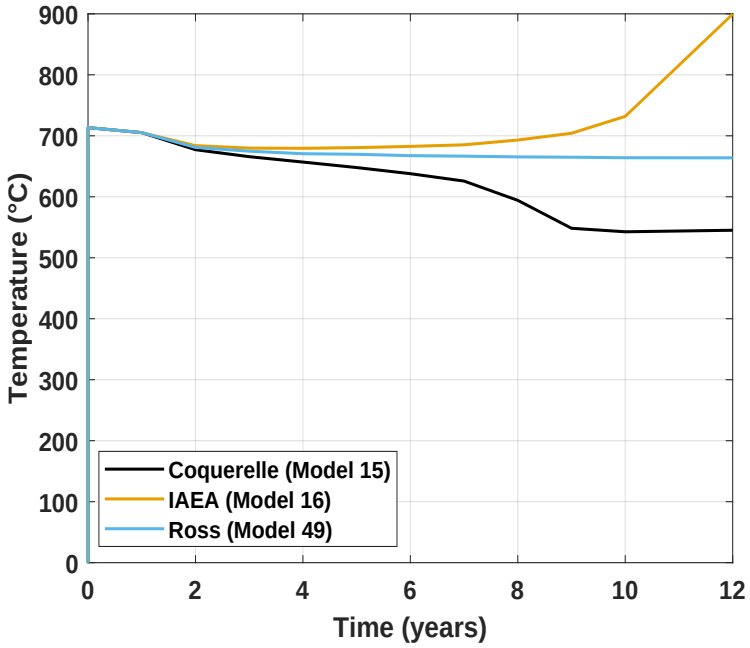


Figure 13: The variation of fuel centre temperature in the swelling models for UN

From the figure above, a clear difference can be observed between the 3 models. This assessment of fuel centre temperature is one of the primary goals of fuel performance modelling as this verifies the accuracy of these calculations that influences the phenomena that are temperature-dependent such as thermal expansion, fission gas release and fuel restructuring. The distinct variation of FCT towards the EOL requires us to look at each of the parameters that the model is affecting, i.e. performing a sensitivity study.

4.3 Sensitivity Study - SWELOC Models

This sensitivity study for the swelling model is done to assess the uncertainties within the models. The assessment is done to check for discrepancies in pressure, gap size, outer fuel radius, fission gas release, fuel stack elongation, gap conductance and various stresses on cladding, including cumulative damage function (CDF). Through these TRANSURANUS simulations, the worst-case can then be characterised by the highest CDF at EOL. The reason for selecting this is that the CDF predominantly relates to the FCMI. On the other hand, the best-case scenario is based on fuel pin experiencing optimal conditions with larger margins to failure for the entire irradiation-induced reactor life.

The three swelling models, i.e the reference (Coquerelle model), the IAEA (model 16) and Ross (model 49), are all individually simulated in TU and subjected to maximum possible reactor operation years without failure. The operating conditions similar to that of Section 4. It was found that the reference model operated until 12 years. In contrast, the IAEA model operated for 15 years and Ross model was operable until 26 years, after which they all reported a cladding rupture failure. Therefore, the following sensitivity study is performed for all three models from BOL until 12 years at full power.

4.3.1 Fuel Centre Temperature Comparison

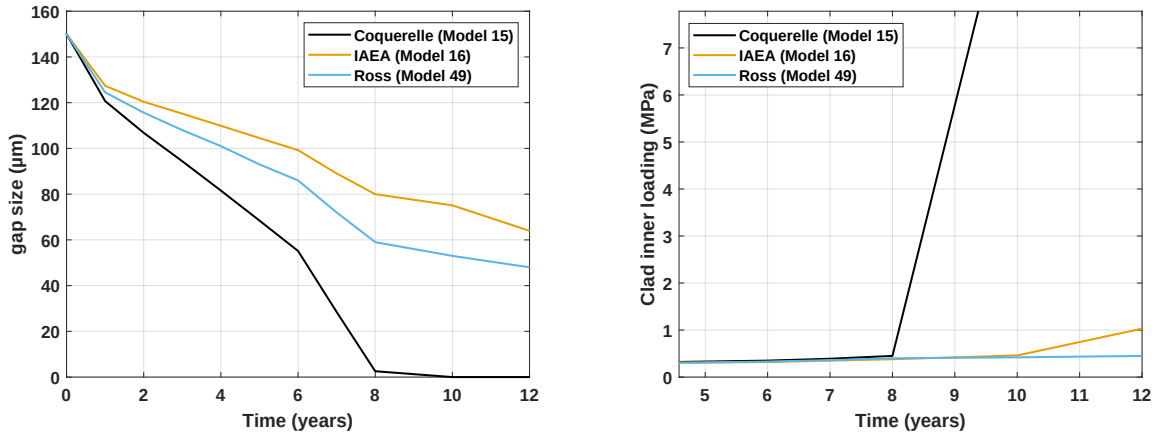
As seen in Figure 13, the Coquerelle model (Reference case) shows a depreciating trend, which might be a consequence due to an increase in gap conductance and gap closure towards EOL. On the other hand, the IAEA model shows a linearly increasing trend towards the 12^{th} year similar to that of the UO_2 fuel (Section 4.1.1); the increase might suggest a substantial FGR associated with it. In contrast, the Ross correlation shows a uniform, coherent trend as the model was operable for 26 years and showed an increasing trend towards its EOL. Table 6 displays the temperature values at 12^{th} year for the 3 models.

Table 6: The temperature values at 12^{th} year for the three swelling models

Temperature	Model
545 °C	Reference Model
900 °C	IAEA Model
663 °C	Ross Model

4.3.2 Contact Pressure and Gap Size

From Figure 14, it can be inferred that the reference model experiences a sharp increase in contact pressure due to gap closure after 10 years of operation. On the other hand, in Figure (14a) the IAEA and Ross Models are very similar in trends and magnitude towards the end of 12^{th} year, as neither of the models experiences a gap closure for this time interval. In Figure (14b), the IAEA model shows a substantially linear increase towards the 11^{th} year, whereas comparatively, the Ross model shows the lowest value in terms of contact pressure. Table 7 displays the variance in contact pressure and gap size values at 12^{th} year.



(a) (b)

Figure 14: Evolution in time of Swelling Models in terms of (a) Gap Size (b) Contact Pressure

Table 7: The clad innerloading and gap size values at 12^{th} year for the 3 models

	Reference Model	IAEA Model	Ross Model
Clad Inner Loading	20.96 MPa	1.03 MPa	0.45 MPa
Gap Size (radial)	0 µm	63.9 µm	48 µm

4.3.3 Fission Gas Release

As seen in Figure 15, the trend for the reference case is justifiable as the fission gas release is mainly caused due to gap closure and increased pressure. Although the IAEA model did not show any gap closure or high pressures like the reference case, it still managed to have a sufficiently large amount of gas release. This maybe due to the increased fuel centre temperature and other factors which might have lead to a drop in thermal conductivity for the filling gas (helium), thereby decreasing the gap conductance resulting in increased amounts of fission gas release into the upper plenum.

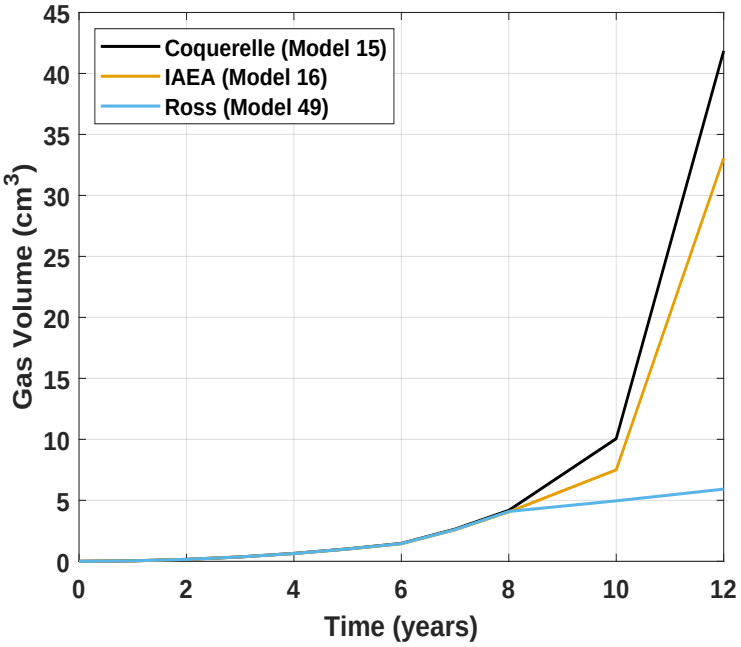


Figure 15: The Variation of fission gas release in swelling models

4.3.4 Gap Conductance

In Figure 16, the reference model displays a significant increase in conductance towards the EOL. On the other hand, the IAEA model experiences a decrease in gap conductance, and this is due to increased amounts of temperature in the fuel; this decrease is further noticeable as the fission gas atoms are released to the open volume. Table 8 displays the variance of gap conductance values of the three models.

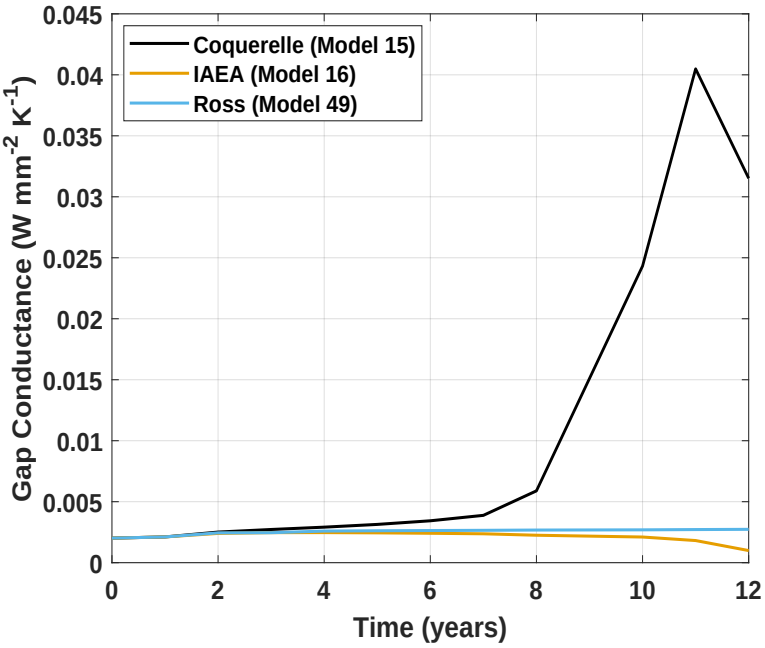


Figure 16: The variation of gap conductance in swelling models at slice 5

Table 8: The gap conductance values at 12^{th} year for the 3 models

Gap Conductance	Model
31516 $Wm^{-2}K^{-1}$	Reference Model
993 $Wm^{-2}K^{-1}$	IAEA Model
2733 $Wm^{-2}K^{-1}$	Ross Model

4.4 Best Case Scenario

Table 9, represents the maximum values in terms of cumulative damage function (CDF) and strains for the cladding with three selected models. The Coqurelle model (reference model) has higher values than the other models, implying that the reference model is the worst-case scenario. However, it need not necessarily be true. The reason for that is that even though the model might be showing higher amounts of CDF, experimental validation might be required. Further narrowing down the selection into the two optional models, both models are assessed to check the main difference between the correlation. The Ross correlation model shows a higher swelling per burnup % at high temperatures (Figure 17 and Figure 18).

Table 9: The maximum values of strain and CDF at 12^{th} year for the 3 models

	Reference Model	IAEA Model	Ross Model
Cumulative Damage Function	0.006	0	0
Permanant Strain %	0.22	0.19	0.19
Irradiation Strain %	0.005	0.003	0.003

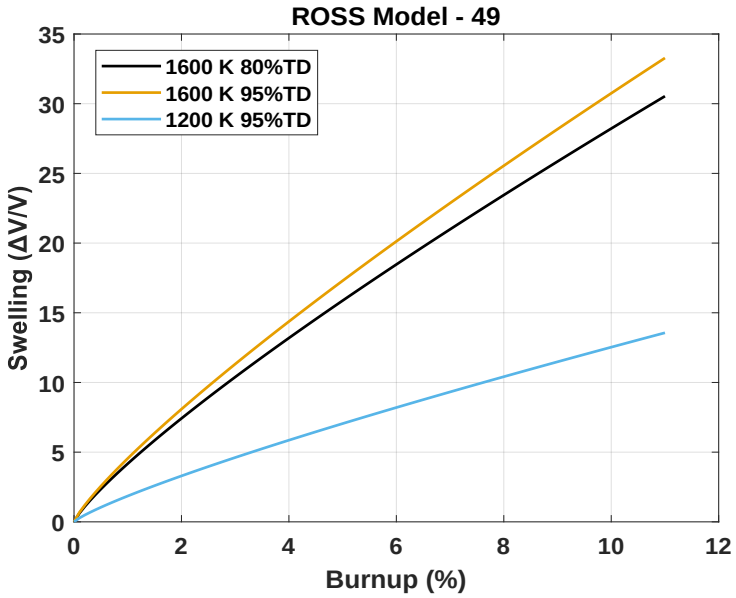


Figure 17: The swelling per burnup% for Ross model

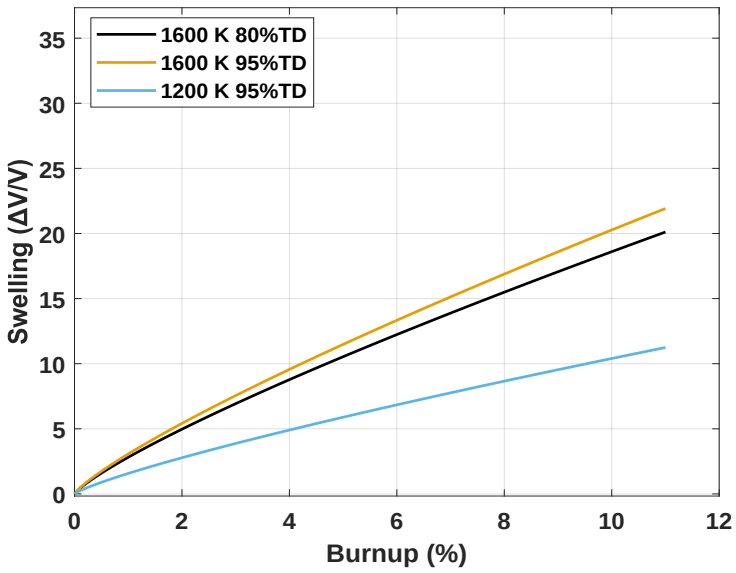


Figure 18: The swelling per burnup% for IAEA model

The three models are affected by high uncertainties throughout the analysis. This inconsistency/variation in the models makes it difficult to predict the best-case scenario for the UN fuel. A table summarizing the variation of the IAEA model and Ross model from the reference case is displayed below (Table 10). Furthermore, in the Ross Correlation (MODEL 49), the fuel tends to operate at relatively moderate temperatures (<750K), showing a potential to operate at higher burnups with low amounts of fission gas release and no failures occurring in the simulation for 26 years. It also shows optimal range values throughout the sensitivity analysis. Thus, indicating that the fuel pin design is very robust. Nevertheless, the prediction of the best-case scenario would be doubtful since the models display such significant uncertainties. Hence a parameter study for the IAEA Model and Ross Model will be performed in the next section.

Table 10: The percent variance between the three models at end of simulation

Phenomenon/Property	Reference Model	IAEA Model	Ross Model
Fuel centre temperature (°C)	545.12	899 (65%)	663 (21%)
Contact pressure (MPa)	20.96	1.03 (95%)	0.45 (97%)
Fuel outer radius (mm)	5.159	5.088 (1.37%)	5.103 (1.05%)
Fission gas release (cm^3)	41.48	33.05 (21%)	5.92 (85%)
Gap conductance ($Wm^{-2}K^{-1}$)	31516	993 (96%)	2733 (91%)
Permanent strain (%)	0.22	0.19 (13%)	0.19 (13%)
Irradiation strain (%)	0.005	0.003 (40%)	0.003 (40%)
Operational years without failure	12	15 (25%)	26 (108%)
Cumulative damage function	0.006	0	0
Gap closure	Occurs at year 10	Not seen	Not seen

5 UNCERTAINTY ANALYSIS

This section aims to evaluate and measure the impact that specific input parameters have concerning fuel performance. The parameter study was carried out through Dakota for IAEA Model and Ross Model. Both the models produced the same results in terms of Spearman correlation coefficients. Hence the results presented in this section are common to both models.

5.1 Selected input parameters

The selection of these uncertain input parameters is based on experience, the recommendations of similar benchmark specifications, expert judgment, access to the parameters (user-specified or source code parameter) and finally, the subject of analysis.

Table 11: Input factors selected for the parameter study

Input file	Description	Type
BETA	Anisotropy factor for densification	Float
Ncracks	Number of cracks in fuel	Integer
Gas_gb	Saturation limit for grain boundary gas	Float
Fmueh	Friction coefficient between fuel and cladding, static	Float
Fmuef	Friction coefficient between fuel and cladding, sliding	Float
Rab	Pellet outer radius	Float
Raubl	Pellet roughness	Float
korngr	Grain diameter	Float
DKORN	Averaged grain diameter for specific creep correlations	Float
openpor	Open porosity	Float
PRODIS	Fraction of dish volume	Float

The selected parameters mentioned in the table above were shortlisted from a broader range as some of the parameters showed no variations in responses/output.

5.2 Variation on input parameters

According to the procedure described in Section 3.2, the input parameters reported in Table 11 were varied uniformly of their nominal values. The uncertainty range is set closest to the maximum allowable range to failure. The selected parameters were varied, so a new set of values for the selected input parameters were obtained. The new set of parameter values were then used

to perform a TU calculation. The procedure was repeated for 512 iterations automatically done by Dakota, resulting in a 512x45 data matrix.

5.3 Ranking of influential parameters

The simulation results were then investigated for the desired output, such as fuel centre temperature. As a result, the iterations produce a varying set of values for all parameters. An example of this varying range can be seen in Table 12 below.

Table 12: Range of iterated values at BOL and EOL

	Range at BOL	Range at EOL
Fuel Centre Temperature °C	640 - 796	554 - 1385
Gap Conductance (W m^{-2} K^{-1})	1439 - 3075	391 - 9111

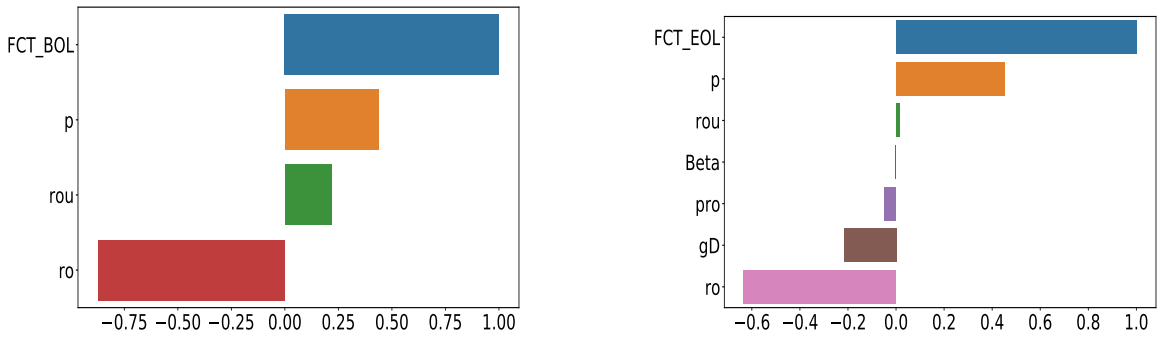
Based on this variation, the inputs certainly influence the output. Thus, after the Dakota simulation is completed, the partial ranked correlation coefficients matrix stored in the Dakota hdf5 file is then accessed to identify the most influential parameters. The Dakota toolkit only allows calculating a statistical index such as Spearman's rank correlations for a Latin Hyper Cube study. Since the study was a multidimensional parameter study, a python script file was used to extract the correlation between the desired output and inputs. The matrix used in this study comprised of 512 cases; thereby improving the confidence level and giving a reasonable P-value associated with the Spearman correlation coefficients.

Table 13: Acronyms used in the uncertainty analysis

Acronym	Description
p	Fuel pellet porosity
rou	Fuel pellet roughness
nC	Number of cracks in fuel
op	Open porosity of fuel
fc1	Friction coefficients
gb	Gas in grain boundary
Beta	Anisotropy factor for densification
pro	Fraction of dish volume
gD	Grain Diameter
ro	Pellet outer radius

5.3.1 Fuel Centre Temperature

Figure 19(a) shows the Spearman correlation coefficients between the fuel centre temperature and selected input parameters at BOL. Here the only significant influential parameter is the ro (outer fuel radius) value with an absolute value of -0.87, indicating an inverse relation with FCT. Implying that if the fuel radius decreases, then the temperature of the fuel at BOL would rise. The other parameters, p (porosity) and rou (fuel pellet roughness) are considered insignificant since they have an absolute value of less than 0.5. Similarly from Figure 19(b) the porosity value is 0.45. Again, it is considered insignificant, whereas the radius having an absolute value of -0.62 indicates an inversely influential parameter for the fuel centre temperature. Here the absolute value of ro decreases at EOL compared to BOL. This is because many other parameters/phenomena also influence the FCT at EOL, such as gap conductance. However, the effect of other parameters/phenomena impacting the subject of analysis was dropped from the study, and only the input influential parameters were assessed.

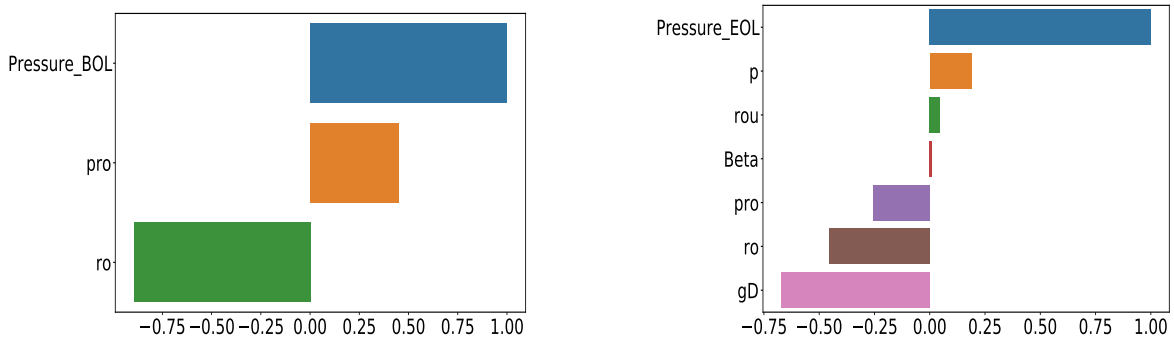


(a) (b)

Figure 19: Spearman correlation coefficients identified between fuel centre temperature and inputs at (a) BOL (b) EOL

5.3.2 Pressure

In Figure 20(a), the Spearman correlations for the clad inner loading at BOL is seen. It can be observed that the pellet radius (ro) inversely influences the pressure at BOL. The other selected input parameters are considered insignificant and not seen. However, at EOL, the absolute value of the correlation coefficient is dominated by the fabrication grain diameter of the fuel pellet (gD), which is inversely related to the clad inner loading. In contrast, the outer fuel radius has a value of just -0.46, becoming irrelevant towards the EOL.

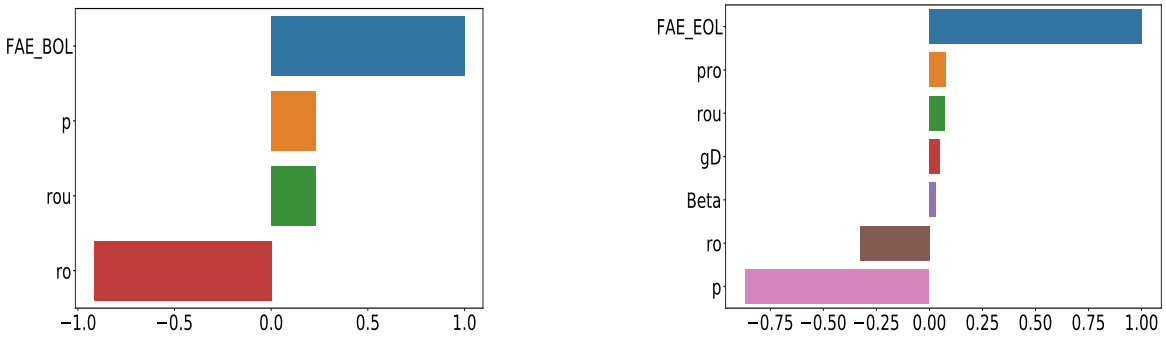


(a) (b)

Figure 20: Spearman correlation coefficients identified between clad inner loading and inputs at (a) BOL (b) EOL

5.3.3 Fuel Axial Elongation

The Spearman correlations coefficients identified at the BOL for fuel axial elongation showed that the pellet radius was the most influential parameter having an inverse relationship with an absolute value of -0.91. In contrast, at the EOL, the dominating factor seems to be the porosity value of the pellet having an inverse relation with the axial fuel elongation with an absolute value of -0.85, indicating that if the porosity of the fuel were increased initially, then the fuel axial elongation would be lower.



(a) (b)

Figure 21: Spearman correlation coefficients identified between Fuel Axial Elongation and inputs at (a) BOL (b) EOL

5.3.4 Fission Gas Release

While identifying the most influential input parameters for the fission gas release with the help of Spearman correlation coefficients (Figure 22), none of the input parameters are considered

significant. Although parameters like porosity, grain diameter and fuel radius showed an absolute value of 0.4, they were still deemed insignificant

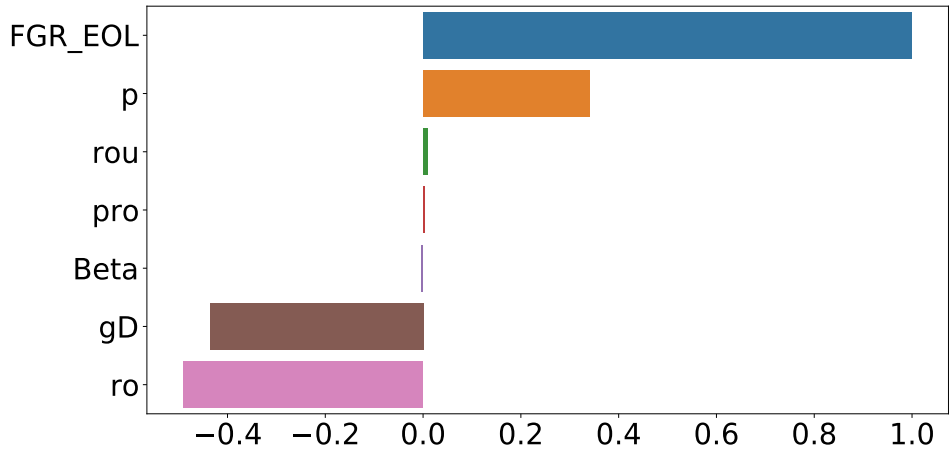
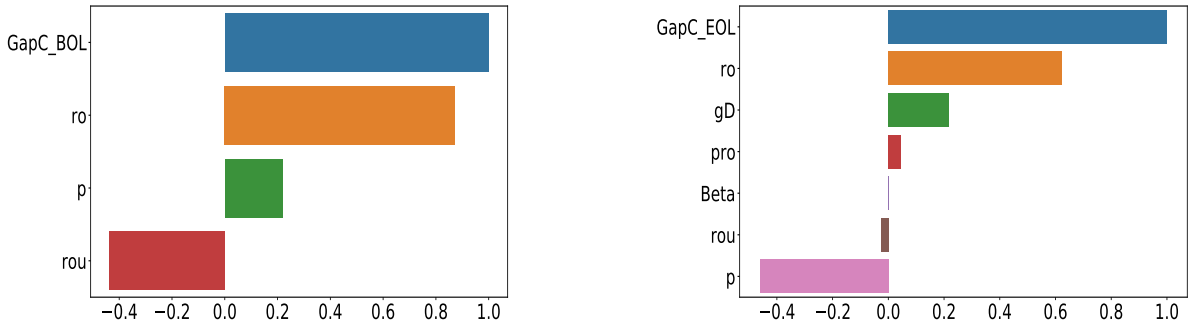


Figure 22: Spearman correlation coefficients identified between FGR and inputs at EOL

5.3.5 Gap Conductance

Identifying the Correlation coefficients for gap conductance, it can be observed that the trends are similar at BOL and EOL. The only parameter of significance is the fuel radius proportional to the gap conductance, implying that an increase in the radius of the fuel will increase the gap conductance.



(a) (b)

Figure 23: Spearman correlation coefficients identified between Gap Conductance and inputs at (a) BOL (b) EOL

6 SUMMARY AND CONCLUSION

6.1 Summary of the work and main conclusions

This thesis work has dealt with SUNRISE LFR fuel pin thermo-mechanical assessment exploiting the TRANSURANUS fuel performance code. By reviewing the models implemented in the TU version V1M1J19, the focus has been on such correlations addressing the fuel behaviour modelling, with the goal to extend the code predicting capabilities for the UN and UO_2 fuel.

The fuel performance analysis was carried out by simulating both the fuels with the most reliable set of input models (reference case). The results for the reference case concluded that both fuels experience a fuel-cladding mechanical interaction (gap closure for UO2 occurring at eight years of irradiation and year 10 for UN). The discrepancy in the trend line for the fuel centre temperature of the UN fuel suggested conducting a sensitivity study to account for the uncertainties associated with modelling key fuel phenomena such as swelling and fuel thermal conductivity. Another sensitivity study further investigated the swelling model to identify correlation sets that make the worst and best case in fuel pin conditions. The scenarios developed have thereby proven a worse case with the highest cumulative damage function to cladding. Although the Ross model simulated a robust fuel pin design that never needed to be replaced during operation, a best-case was not established. The reason is due to large uncertainties within the models, lack of experimental data to validate, and minimal design limits that were set.

The uncertainty analysis was achieved by making use of Dakota. The software allows the generation of random samples for a set of input parameters of interest. By coupling the Dakota tool with TRANSURANUS, the TU calculation was modified according to the variation of input parameters. Furthermore, the software allowed multiple TU simulations based on the variation of the input parameters, generating a data matrix consisting of the partial ranked correlation coefficients for the selected input parameters. Results from the data matrix are then extracted by a python script that gives the desired plots rendering the Spearman correlations coefficients for the selected parameters.

Some of the influential input parameters did appear significant to the uncertainty study. However, the IAEA and Ross model both displayed the same values of Spearman correlation coefficients, thus implying that it need not be so critical to assess the fuel pellet's design but rather indicative towards a better understanding of the theoretical swelling model for the Uranium Nitride fuel. Furthermore, the IAEA model displays an unusual trend with gap

conductivity lowering; this indirectly hints at a newer gap conductance model being developed and tested that considers a contact pressure term between the fuel and cladding[28].

6.2 Future work

Some recommendations for the future work can be summarized based on the work presented in the thesis.

The available irradiation data for the Uranium Nitride fuel is scarce and very old, limiting the analysis's extent. Moreover, the fuel-dependent models must be updated in the fuel performance code, which is extensive and complicated. Nevertheless, common developments to the fuel performance code by the users and international benchmarking would enable the dissemination of knowledge gained and improvement of fuel performance modelling.

Furthermore, exercising the iterative process of separate effects testing with advanced modelling and simulations could substantially accelerate fuel development.

The partial rank correlation coefficients are a linear association between an input and an output. Therefore, additional sensitivity methods could be employed further to investigate the variability of the output with input—for example, the Sobol method.

Since experimental data is unavailable, the influential input parameters may have other uncertainties; therefore, testing different probability distributions functions could be beneficial.

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APPENDIX

Table 14: Recommended fuel specific model properties implemented in TU for UN fuel. The correlations for all models can be found in the TU manual [20]

Model	Input file
Creep aniso (Anisotrp)	ModFuel(1)=15
Elasticity constant, (ELOC)	ModFuel(2)=15
Poisson's ratio, (NUELOC)	ModFuel(3)=15
Strain due to swelling, (SWELOC)	ModFuel(4)=15
Thermal strain (THSTRN)	ModFuel(5)=15
Thermal conductivity (LAMBDA)	ModFuel(6)=15
Creep strain (ETACR)	ModFuel(7)=15
Yield stress (SIGSS)	ModFuel(8)=15
Rupture strain (ETAPRR)	ModFuel(9)=15
Fraction of heavy metal (ANSWME)	ModFuel(10)=15
Specific heat at constant (CP)	ModFuel(11)=15
Density (RO)	ModFuel(12)=15
Solidus liquidus melt temperature, (SOLIMT)	ModFuel(13)=15
Heat of evaporation, (FH)	ModFuel(14)=15
Emissivity (EMISS)	ModFuel(15)=15

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