Modeling and Simulation Needs and Capabilities for Artificial Intelligence Based Plant Reload Optimization Platform

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Abstract: The Risk-Informed Systems Analysis (RISA) Pathway Plant Reload Optimization Project under the United States (U.S.) Department of Energy's (DOE's) Light Water Reactor Sustainability (LWRS) Program—aims to develop and demonstrate an automatized technology-inclusive platform that can generate optimized fuel load configurations for the reactor core of a nuclear power plant. The project targets to optimize reactor core thermal limits through the implementation of state-of-the-art computational and modeling techniques. During the development of the platform, the constraints were identified in computational tools. The main issue that was identified is that the tools need to be immediately applied to the optimization platform without significant development or update. The tools used in the platform should have the highest technical maturity so that they can be deployed to nuclear industry with ease. Hence, this study focused on reviewing the applicable computational tools in the field of the reactor core design and fuel performance analysis to give a snapshot on tool selection for the optimization platform. The benchmark study was therefore performed using well-designed case studies for the core design and fuel performance tools planned to be used in the plant fuel reload optimization framework. Three core design tools-VERA-CS, SIMULATE-3, and PARCS-are reviewed and compared with different hot zero power tests, physical reactor zero power physics tests, and a hot full power case. Two fuel performance tools-BISON and TRANSURANUS-are reviewed and compared with two instrumented fuel assembly test cases to analyze fuel performance under the long-term operation and loss of coolant accident event. Other parameters are benchmarked, including computational performance issues while coupling with Risk Analysis and Virtual Environment (RAVEN) and accident tolerance fuel (ATF) applicability.

1. INTRODUCTION

The Risk-Informed Systems Analysis (RISA) Pathway Plant Reload Optimization Project —under the United States (U.S.) Department of Energy's (DOE's) Light Water Reactor Sustainability (LWRS) Program aims to develop an integrated, comprehensive platform offering an all-in-one solution for the reload evaluations with the special focus on fuel optimization, which allows a reduction in the volume of new fuel [1]. The platform will provide an optimized reactor core configuration based on key safety parameters that must be considered to meet regulatory requirements. The optimization methods are at the core of the framework, which can search in the enormous design space for the optimal loading pattern with maximized fuel utilization and improved safety limits by leveraging modern core/system modeling and simulation capabilities. It is, however, constraint in the computational tools that have been identified during past activities of the project, especially in the field of reactor core design and fuel performance codes. The optimization framework uses an artificial intelligence (AI)-based genetic algorithm (GA) and requires hundreds to thousands of calculations even with a reduced-order model. For this reason, computational economics became one of most important parameters while developing an optimization framework.

A benchmark study was conducted for a comparison study of reactor core design and fuel performance computer codes to determine tool capability and applicability for the fuel reload optimization framework. Figure 1 shows a schematic diagram of the plant fuel reload optimization framework. The

framework has three different areas: core design, fuel performance and system analysis. The Reactor Excursion and Leak Analysis Program (RELAP) 5-3D code was selected as the best-estimate system analysis code. It is fully validated and versatile to be tightly coupled with Risk Analysis and Virtual Environment (RAVEN), which is the main operating tool for the optimization platform. The core design and fuel performance tools still need a comprehensive applicability review for this platform. For the core design tools, different codes are considered from newer high-fidelity codes to more established codes used in the nuclear industry and regulatory body. From multiple tools available three most appropriate for the platform are selected for a detailed comparison: VERA-CS, SIMULATE-3, and PARCS. The aspects of the investigated performance of these codes include the time-dependent simulation capability, computational efficiency, integration with upstream cross-section generation modules, user-friendliness, etc. For the fuel performance tools, two codes are evaluated-TRANSURANUS and BISON. The benchmark uses two test cases developed and described by the Organization for Economic Co-operation and Development (OECD)/Nuclear Energy Agency's (NEA's) International Fuel Performance Experiments (IFPE): (1) the Instrumented Fuel Assembly (IFA)-432 Rod 3 case is used to evaluate fuel performance during long-term operation; and (2) the IFA-650.2 Rod 2 case is used to analyze fuel failure mechanism during a loss of coolant accident (LOCA).

Figure 1: Schematic Diagram of Plant Reload Optimization Platform.



The benchmark results were assessed for applicability to the optimization framework. The main criteria for tool selection include:

- <u>Computational Speed</u>: Optimization algorithm (e.g., GA) requires a minimum order of hundreds of simulations. Hence, the tools need to be run as fast as possible, preferably on the order of a tenth of a second.
- <u>Higher Technical Maturity</u>: Optimization framework aims at immediate industrial deployment. The tools under the framework need to have at least higher than TRL level 7.*
- <u>Coupling with RAVEN</u>: RAVEN is the main software to control the optimization platform. Though RAVEN has a high degree of freedom, code coupling with RAVEN needs to be verified.
- <u>Accident Tolerant Fuel (ATF) and/or High-Burnup</u>: The tools under the optimization framework need to address the capability to apply both ATF and high-burnup operation.
- <u>Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR)</u>: The tools under the optimization framework need to be applicable for both PWR and BWR.

^{*} TRL is from 1 to 9, Level 7 is the minimum requirement for actual demonstration, https://www.nasa.gov/directorates/heo/scan/engineering/technology/technology_readiness_level.

2. CORE DESIGN TOOL BENCHMARK

Three core design tools—VERA-CS, SIMULATE, and PARCS—were used for the benchmark. The primary parameter of interest is code performance, including the simulation capability, computational efficiency, integration with upstream cross-section generation modules, and user friendliness, as well as ATF applicability. The controlled benchmark calculations for this purpose are three exercises in the Watts Bar Unit 1 (WB1) multi-physics benchmark with a focus on two main exercises: stand-alone 3D neutronics model at hot zero power (HZP) conditions and multi-physics steady-state model for hot full power (HFP) conditions at the beginning of cycle (BOC) [2]. The problems will identify optimal code capabilities by performing different multi-scale calculations from the pin cell up to full core HZP and HFP operating conditions.

Generally, for core design, the two-step method has been used in steady-state and transient core analysis: lattice physics calculation to develop few-group homogenized cross-section of each fuel assembly based on reactor conditions; and few-group nodal diffusion-based coupled neutronics/thermal-hydraulics calculations for reactor power and other important parameters. Recently, one-step method has been developed based on high-fidelity advanced solvers and multi-physics coupling algorithms for explicit pin-by-pin transport solutions. Comparing these two methods, one notable difference is the computational runtime. A full set of lattice physics calculations for the twostep method has the significant advantages of simulation time and computational resources. This clearly indicates that the two-step method will be a better option for AI-based optimization and perturbation studies.

2.1. Description of Selected Core Design Tools

The VERA-CS simulation environment was developed by the Consortium for Advanced Simulation of Light Water Reactors (CASL) for the direct multi-physics coupling of existing high-fidelity physics code with capabilities for transient neutron transport, thermal-hydraulics, fuel performance, and chemistry calculations [3]. The code is optimized for spatial fidelity with an emphasis on performance and parallelization. The VERA-CS reactor simulation application includes the subset of these coupled physics codes needed for reactor core depletion over multiple cycles.

SIMULATE is an advanced three-dimensional two-group nodal code for the analysis of both PWRs and BWRs [4]. The SIMULATE generally use together with CASMO multi-group two-dimensional fuel assembly burnup calculation code for the use of PWR and BWR fuel depletion. This code can be run in partial, full, or multi-assembly geometry and produce two-group homogenized cross-sections for use as the SIMULATE input. SIMULATE can apply thermal-hydraulic feedback by calculating a 3D fuel temperature from an average fuel pin temperature and coolant temperature as a boundary condition. The code also allows for the use of pre-computed temperature tables and accounts for physical changes, such as thermal expansion, irradiation-induced swelling of the fuel, and fuel pellet cracking with burnup by adjusting the conductivity of fuel and cladding.

The Polaris/PARCS computational suite includes Polaris, the 2D lattice physics code; and PARCS, the neutronics calculation code [5]. Developed by Oak Ridge National Laboratory (ORNL), Polaris aims to be used in light water reactors (LWRs) by a transport solver together with the embedded self-shielding method to condense and homogenize the cross-sections. PARCS is the core neutronics code supported by the U.S. Nuclear Regulatory Commission (NRC) and is primarily used for modeling LWRs for steady state, depletion, and transient calculations. PARCS solves the time-dependent two-group nodal diffusion equations. The pin power reconstruction capability can be used to provide pin-by-pin power information. Beyond diffusion problems, PARCS can compute thermal-hydraulic feedback using two different solvers.

2.2. Core Design Tool Benchmark

Figure 2 shows a 2D image of the WBN1 cycle 1 full core layout on the left with an axial layout of the fuel assembly on the right. The axial layout includes the upper and lower core plates, nozzles, gaps, Inconel and Zircaloy spacer grids.





The WBN1 reactor core contains 12-foot tall 193 fuel assemblies in a 17×17 assembly, including 264 fuel rods, 24 guide tubes, and one central instrumentation tube. The reactor core is loaded with three regions of fuel assemblies with specific enrichments of 2.11%, 2.619%, and 3.10%. Table 1 provides the core operating conditions and design parameters of these assemblies. Five benchmark cases were considered based on the standard VERA-CS Table 1: Core Operating Conditions and

validation suite and used as reference data [6]:

- Case 1: 2D eigenvalue lattice problem at HZP BOC
- Case 2: 2D central core assembly lattice problem at HZP BOC
- Case 3: 2D fuel assembly interface and control rod effect lattice problem at HZP BOC
- Case 4: Zero Power Physics Tests (ZPPTs) of reactor core problem
- Case 5: 3D reactor problem at HFP BOC.

2.2.1. Case 1: 2D Eigenvalue Lattice Problem at HZP BOC

Table 1: Core Operating Conditions and
Design Parameters.

Description	Value
Rated Core Power (MW)	3411
Reactor System Pressure (MPa)	15.51
Coolant Inlet Temperature (K)	565
Coolant Core Bypass Flow Rate (%)	9
Cycle 1 HZP BOC ARO Critical Soluble Boron Concentration (ppm)	1291
RCCA Control Bank Overlap (steps)	128
Cycle 1 Uranium Fuel Loading (MT)	88.808
Rated Coolant Total Flow Rate (kg/s)	18231.89
Cycle 1 EOC Exposure (GWd/MT)	16.939

This case demonstrates the code capability of solving a simple 2D pin cell eigenvalue problem. Five tests are performed within a different range of moderator and fuel temperatures, as well as the moderator

density in the full operating isothermal conditions of zero power condition. Table 2 shows the Case 1 tests specification and results of effective multiplication factor (k_{eff}) comparison. Results are all comparable to reference data. Maximum difference was found in VETA at test 1E, which includes the Integral Fuel Burnable Absorber (IFBA) model.

2.2.2. Case 2: 2D Central Core Assembly Lattice Problem at HZP BOC

The Case 2 demonstrates code capability of a simple 2D central assembly fuel road array. Three cases with change in enrichment and fuel and moderator temperatures are tested. Table 3 shows benchmark specification and results. Figure 3 shows the pin power distribution difference compared to reference value. No significant discrepancy was found between reference and simulation.

	Specifications				Results (<i>k_{eff}</i>)				
Test	Moderator Temperature (K)	Fuel Temperature (K)	Moderator Density (g/cm ³)	Reference (ENDF/B- VII.0)	Reference (ENDF/B- VI.8)	VERA- CS	Polaris- HiFi	CASMO	
1A	565	565	0.743	1.18704	1.18336	1.18704	1.18643	1.18428	
1B	600	600	0.661	1.18215	1.17855	1.18221	1.18194	1.17952	
1C	600	900	0.661	1.17172	1.16811	1.17165	1.17166	1.16927	
1D	600	1200	0.661	1.16260	1.15922	1.16285	1.16283	1.16015	
1E	600	600	0.661	0.77169	0.77033	0.76966	0.77144	0.77159	

Table 2: Benchmark Case 1 Specifications and Results (k_{eff}) .

Table 3: Benchmark	Case 2 Specifications	and Results (k _{eff}).
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		Results (<i>k_{eff}</i>)						
Test	Specifications	Reference (ENDF/B-VII.0)	Reference (ENDF/B-VI.8)VERA-CS		Polaris-HiFi	CASMO		
2A	3.1w/o	1.182175	1.17852	1.1822784	1.18112	1.17824		
2B	600K	1.069627	1.066596	1.0706106	1.068157	1.06718		
2C	600K	0.976018	0.973376	0.9775254	0.97471	0.97416		

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Table 4: Cross-sections from the Case 3 Results.

	Pola	aris	CASMO		
	G1	G2	G1	G2	
Total	6.47E-01	1.87E+00	6.70E-01	1.90E+00	
Absorption	2.06E-03	4.13E-02	2.70E-03	4.27E-02	
NuFission	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
Diff. Coefficient	1.32E+00	2.78E-01	1.19E+00	2.70E-01	
In Scattering	6.14E-01	1.83E+00	6.42E-01	1.85E+00	
Out Scattering	3.16E-02	7.04E-04	2.58E-02	1.01E-03	

2.2.3. Case 3: 2D Fuel Assembly Interface and Control Rod Effect Lattice Problem at HZP BOC

The Case 3 investigates the fuel assembly interfaces and control rod effects in 2D. Core response is tested with two-group cross-sections. The geometry of this case includes 0.19 cm of the fuel baffle gap and 2.85 cm of the baffle thickness. Results are shown in Table 4. No significant discrepancy was found. This case was only performed for the Polaris and CASMO codes, since the VERA-CS uses a multi-group cross-section in default.

2.2.4. Case 4: ZPPT of Reactor Core Problem

Case 4 is a typical HZP isothermal condition reactor case to assess the radial and axial power profile. The test includes demonstration of the eigenvalue and core reactivity coefficients without thermalhydraulic feedback or depletion. Figure 4 shows the core average axial power profile. The three code results are in good agreement. For the VERA-CS result, the power profile shows peaks where the core structure (e.g., spacer grids) was simulated. Figure 5 shows the radial power profile distribution from code-to-code benchmark with VERA-CS, SIMULATE, and PARCS by using relative difference (%). The result from PARCS shows a maximum of 7.8% and 3.6% from SIMULATE.





Figure 5: Case 4 Radial Power Comparison with VERA-CS to SIMULATE (left) and PARCS (right).



Figure 6: Core Average Axial Power (left), Fuel Temperature (center), and Moderator Density (right) Profile in Benchmark Case 4.



2.2.5. Case 5: 3D Reactor Problem at HFP BOC

Case 5 demonstrates a typical operating reactor with nominal power and flow conditions. The simulation condition includes equilibrium xenon isotopes and critical soluble boron with thermalhydraulic feedback to the neutronics in fuel and coolant. Figure 6 shows the core average axial power, fuel, and moderator temperature profile. The three code results are in good agreement. As with the previous test, the VERA-CS result showed an existing peak core structure. Figure 7 shows the radial power profile distribution from code-to-code benchmark with VERA-CS, SIMULATE, and PARCS by using relative difference (%). No significant differences were identified.



Figure 7: Case 5 Radial Power Comparison with VERA-CS to SIMULATE (left) and PARCS (right).

Table 5: Comparison of Core Design Tool Compu	tational Time (hh:mm:ss; NA: not available).
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Benchmark	VERA-CS	Polaris/PARCS	CASMO-4/SIMULATE-3
Case 1	0:00:02	0:00:11/NA	0:00:01/NA
Case 2	NA	0:01:00/NA	0:00:05/NA
Case 3	NA	0:55:00/NA	0:00:35/NA
Case 4	20:44:15	01:30:00/0:00:02	0:11:05/0:00:14
Case 5	45:01:14	01:30:00/0:00:02	0:11:17/0:00:07

2.3. Core Design Tools Computational Performance Comparison

The three codes provided good results in the entire benchmark test cases. The SIMULATE-3 code uses ENDF/B-VI.8 nuclear data while VERA-CS and PARCS uses a relatively newer version,

ENDF/B-VII.0, but did not observe any significant discrepancy in the results. Since VERA-CS includes a sub-channel and fuel pin model, the axial power profile showed the effect of a spacer grid. However, the simulation time of VERA-CS is incomparable with the other two codes. As shown in Table 5, the computational time of VERA-CS is too long though the code provides high-fidelity outcomes.

3. FUEL PERFORMANCE TOOL BENCHMARK

Two fuel performance tools—TRANSURANUS and BISON—were used for the benchmark. As with the core design tool benchmark, the main parameter of interest is simulation time capability, computational efficiency, integration with the plant reload optimization framework—including RAVEN and RELAP5-3D, and user friendliness, as well as ATF applicability. Two well-controlled benchmark cases were used: (1) IFA-432 Rod 3; and (2) IFA-650.2 Rod 2 of OECD/NEA's IFPE program, which is a public database on nuclear fuel performance experiments for the purpose of code development and validation [7]. These test sets were used for BISON code validation. The IFPE program aims to provide a comprehensive and well-qualified database on Zr clad UO₂ fuel for model development and code validation in the public domain. The data encompasses both normal and off-normal operation and includes prototypic commercial irradiations, as well as experiments performed in material testing reactors. This work is carried out in close cooperation and coordination between OECD/NEA, the International Atomic Energy Agency (IAEA), and the NEA Halden Reactor Project.

3.1. Description of Selected Fuel Performance Tools

TRANSURANUS is a fuel performance code developed at the Joint Research Centre's Institute for Transuranium Elements in Karlsruhe, Germany [8]. The code approximates the fuel rod behavior with an axisymmetric, axially stacked, one-dimensional radial representation. The code can be employed for both steady-state and transient analyses and incorporates models accounting for the different and interrelated phenomena occurring in the fuel rod. The TRANSURANUS code can deal with a wide range of different situations, as given in experiments, under normal, off-normal, and accident conditions. The time-scale of the problems to be treated may range from milliseconds to years. The code has a comprehensive material data bank for oxide, mixed oxide, carbide, and nitride fuels, zircaloy, and steel claddings, in addition to several different coolants.

Developed by Idaho National Laboratory (INL), BISON is a high-fidelity, finite element-based nuclear fuel performance analysis code applicable to a variety of fuel forms, including LWR fuel rods, tri-structural isotropic (TRISO) particle fuel, and metallic rod and plate fuel [9]. BISON solves the fully-coupled thermo-mechanics and species diffusion for various multi-dimensional problems. Fuel models describe temperature and burnup dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. Plasticity, irradiation growth, and thermal and irradiation creep models are implemented for clad material behavior. Models are also capable to simulate gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, gas temperature, and fission gas addition. BISON is based on the MOOSE framework and can therefore efficiently solve problems using standard workstations or very large high-performance computers.

3.2. Fuel Performance Tool Benchmark

Two test sets were selected from BISON standard validation suites [9]: IFA-432 test for fuel performance at long-term LWR operation and IFA-650.2 test for fuel failure mechanism during LOCA.

3.2.1. Halden IFA-432 Rod 3 Test

The main objectives of IFA-432 were measurements of fuel temperature response, fission gas release, and mechanical interaction on BWR-type fuel rods up to high-burnup. The major figure of merit is fuel centerline temperature. During the Halden reactor experiment, the fission gas release threshold was not

excessed, except at the peak power position near 28 MWd/kg UO₂. Rod 3 achieved a burnup of approximately 45 MWd/kg U. Rod 3 also experienced power ramps in the range of 30-45 kW/m. Fuel temperatures at constant power increased steadily throughout the test. During the test, the measured maximum temperature was 1800 C°. The measured lower-level thermocouple temperatures remained below 1300 C°.

The benchmark mainly focused on code capability for predicting fuel centerline temperature. Only the TRANSURANUS simulation was performed and compared with experimental data for a total of 70,000 hours. The BISON simulation was not performed due to the expected simulation running time of more than 30 days. The TRANSURANUS simulation generally agrees with experimental data. The left side of Figure 8 is the centerline temperature during the entire lifetime. Both the experiment and TRANSURANUS simulation results are very much overlapped, and it is not easy to understand the difference. Hence, the ratio between the TRANSURANUS simulation and experimental data is shown on the right side of Figure 8. It was found that the TRANSURANUS simulation slightly over-estimates the centerline temperature mostly at a higher temperature range.





3.2.2. Halden IFA-650.2 Rod 2

Also performed at the Halden reactor, the IFA-650 tests are the series of integral in-pile experiments to investigate fuel behavior under LOCA conditions. The IFA-650 tests focused on embrittlement and mechanical properties of high-burnup cladding. The IFA-650 test series is one of the important experiments to support the high-burnup fuel design and test of new cladding material verification and validation (V&V) during LOCA. The Rod 2 test focused on ballooning and fuel failure to find out how to run the later experiments with the pre-irradiated rods. The test was carried out using a fresh, pressurized PWR rod and low fission power to achieve the desired temperature conditions. The target peak cladding temperature (PCT) of 1050°C was reached and the clad ballooning and rupture occurred at ~800°C.

Both TRANURANUS and BISON were used for the IFA-650.2 Rod 2 test to evaluate rod burst (e.g., ballooning and failure) during the LOCA scenario. The test was carried out using low fission power to achieve the desired conditions for ballooning. Fuel failure occurs due to fuel rod overheating during LOCA and continuous mechanical loading to the fuel rod induces large plastic deformation and burst of the cladding. The main cause of fuel rod burst is rod internal pressure (RIP), as shown in Figure 9. The RIP increases as the LOCA event starts from time 0-seconds. The RIP increases until 7MPa and blowdown to ambient pressure near 61 hours of simulation time, which represents fuel rod burst. These phenomena are clearly observed in both TRANSURANUS and BISON simulations. It is noted that the experimental pressure gauge instrument has a lower measuring limit of 5.5MPa, while the experiment

data line (e.g., orange in Figure 8) does not show smaller than 5.5 MPa. Compared to TRANSURANUS, BISON under-predicts pressure during the simulation. The fuel burst time is within 0.1 seconds between the experiment and both simulations.





3.3. Fuel Performance Tools Computational Performance Comparison

The simulation times for both IFA-432 and IFA-650.2 were longer than expected to meet the level of detail from the experiment data. Table 6 shows the computational time comparison for both TRANSURANUS and BISON. BISON was run using the INL high-performance computing (HPC) cluster with 32 computer processors. The BISON IFA-432 Rod 3 test case only includes the first 8 hours of transient while the entire experiment includes data for 70,000 hours. Considering BISON can simulate 1 hour in about 50 seconds of running time, 70,000 hours will need more than 30 days of running time. Hence, no additional BISON simulation was conducted for the IFA-432 Rod 3 test. It is noted that the generic fuel reload licensing analysis has an order of 100 timesteps, which takes a few seconds of run time if TRANSURANUS is used.

	1	TRANSURANUS	BISON			
Test Case	Operating System	Run Time (s)	Time Steps	Operating System	Run Time (s)	
IFA-432 Rod 3	Windows	27.629	14695	T :	6030	
	Linux	54.239	14085	Linux	(incomplete)	
IFA-650.2 Rod 2	Windows	19.483	3001	2001	Linux	400.8
	Linux	37.998		Linux	409.8	

 Table 6: Comparison of fuel performance tool computational time.

4. CONCLUSION

The main purpose of this activity was to review available computational tools to be used in the plant reload optimization framework. The selection of the tools is purely based on their applicability to the optimization framework. The main criteria of tool selection are as follows.

For the core design tool, the results of this study demonstrated that the two-step approach to core simulation and reactor analysis is more favorable to optimization studies than its one-step counterpart. This is due to the ease of core simulation repeatability for this approach. CASMO/SIMULATE has an ATF modelling feature. As a result, CASMO/SIMULATE is the best option for the optimization framework in terms of above criteria except coupling with RAVEN, which will be completed in 2022.

For the fuel performance analysis tool, TRANSURANUS has a higher advantage in terms of simulation time, which shows more than a hundred times faster than BISON while requiring comparably lighter computational resources. The fast execution time of TRANSURANUS also eliminates the need for simulating with the reduced order models. TRANSURANUS and BISON can model ATF. However, TRANSURANUS needs coupling with RAVEN, which also will be done in 2022.

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