

HIGH FIDELITY AND REDUCED ORDER SOLUTIONS TO AN SMR-LEVEL PROGRESSION PROBLEM WITH THE KRAKEN COMPUTATIONAL FRAMEWORK

Ville Valtavirta, Unna Lauranto, Ville Hovi, Jussi Peltonen,
Antti Rintala, Riku Tuominen, Jaakko Leppänen
VTT Technical Research Centre of Finland Ltd
P.O. Box 1000, FI-02044 VTT, FINLAND
ville.valtavirta@vtt.fi

ABSTRACT

Kraken is a new computational reactor analysis framework under development at VTT Technical Research Center of Finland Ltd. The framework builds heavily on the new generation of Finnish simulation codes such as the Serpent Monte Carlo code, the Ants nodal neutronics solver and the FINIX fuel behavior module.

This paper describes the application of Kraken to its first realistic full core problem, a small modular reactor (SMR) core in its fresh state in order to evaluate control rod worths, shutdown margins and reactivity coefficients for the core.

KEYWORDS: Kraken, SMR, shutdown margin, reactivity coefficient, reactivity worth

1. INTRODUCTION

The Kraken reactor analysis framework [1] ties together various novel Finnish reactor analysis tools in a modular fashion. Neutronics, thermal-hydraulics and thermal-mechanics solvers are coupled via a central multi-physics driver forming a core analysis tool that can be later coupled to system codes via a separate interface to model transients with power plant level feedbacks. While one of the main goals of the framework is to leverage Finnish reactor analysis tools and build new source code level expertise through their development, coupling and use, coupling to state-of-the-art third-party solvers is also supported.

In this article we use two different calculation sequences where the neutronics is solved either using the Monte Carlo code Serpent or the nodal neutronics solver Ants. In both cases, the thermal hydraulics are solved with Kharon, a steady-state closed-channel porous-medium two-phase thermal-hydraulics solver, while the fuel behavior is solved using SuperFINIX. A short introduction of the different modules is given in the next section.

2. COMPUTATIONAL TOOLS

The **Serpent** Monte Carlo code [2] has been developed at VTT since 2004. Originally, Serpent was developed for reactor physics applications and while its applications have significantly diversified over the years, reactor physics remains as the main development direction of the code. Serpent serves in a dual role in the Kraken framework both producing group constants for reduced order solvers and providing direct high-fidelity neutronics solutions in coupled problems. As the

group constants and the full 3D solution can be obtained using the same transport code and the same nuclear data libraries, Serpent is able to provide the best possible reference solution for the frameworks reduced order solvers.

The **Ants** nodal neutronics solver [3,4] has been developed at VTT since 2017 and currently solves the time-independent multi-group diffusion equation in rectangular and hexagonal geometries using a hybrid of the AFEN and FENM methods. Designed to be a robust multi-group code, Ants will serve as the go-to reduced order solver in the framework regardless of the reactor type.

The **FINIX** fuel behavior module has been developed at VTT since 2012 [5]. FINIX solves the behavior of a single fuel rod in base irradiation and transient scenarios and has models for thermal-mechanical behavior of the fuel rod under transient conditions and extended irradiation periods.

The **SuperFINIX** module [6] handles the core level fuel behavior solution and serves as a wrapper for a large number individual FINIX solvers that represent the unique fuel rods in the geometry.

Kharon is a simple thermal hydraulics code meant to serve as a simplified solver for the multi-physics coupling and in educational use while more advanced solvers are developed. Being a closed channel two-phase steady state solver based on the porous medium approach its applications are limited to time-independent simulations with a closed assembly geometry or no appreciable cross-flows.

Cerberus is the multi-physics driver module of the Kraken framework. The individual solver modules communicate with Cerberus via sockets with Cerberus handling the field transfers and solver execution.

3. PROBLEM DESCRIPTION

The first progression problem for the framework as a whole was the simulation of a 3x3 assembly 3D colorset geometry in Ref. [1]. This initial problem simply tested the communication and field transfers between the different solvers and the multi-physics driver as well as the use of Serpent as a computational benchmark to the reduced order neutronics solution. The first progression problem was simplified in many important ways:

- No reflector modeling. The system was radially infinite with axially black boundary conditions at the ends of the active fuel.
- No equilibrium xenon modelling.
- No spacer grids.
- No control rods.

This SMR scale progression problem adds those missing elements to the modeling. Furthermore, this problem tests the application of Kraken to evaluating licensing relevant reactor physical parameters such as control rod worths, shutdown margin and core reactivity coefficients.

3.1. Core Model

The SMR core is based on a combination of data from the NuScale licensing documents [7] and the BEAVRS benchmark [8]. The general core size of 37 fuel assemblies with an active length of 200 cm as well as the radial heavy reflector are based on the NuScale data, whereas the fuel assembly and control assembly designs are based on the BEAVRS benchmark along with their material definitions. The length of the fuel and control assemblies has been reduced in order to match the 200 cm active fuel length in the NuScale concept.

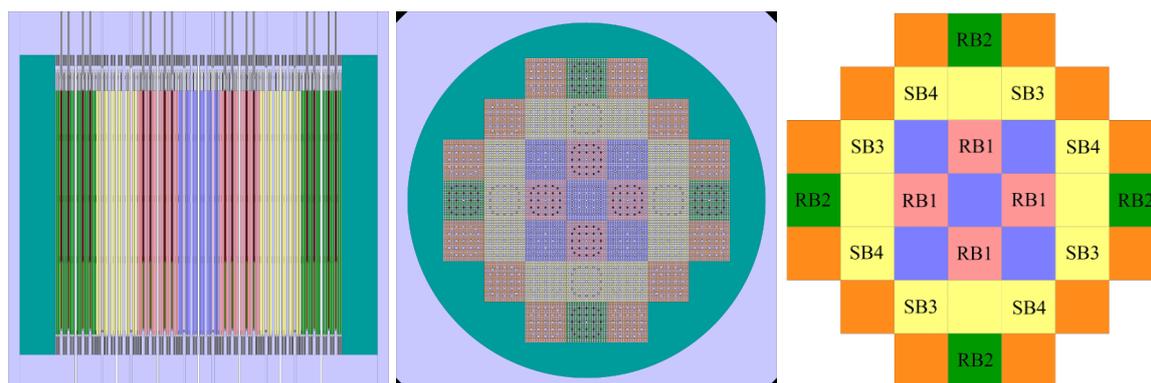


Figure 1: Serpent geometry plots of the modelled SMR core (left and middle) and the naming of the different control rod groups (right).

Fig. 1 shows horizontal and vertical geometry plots of the modelled core geometry as well as the positioning of the four control rod groups: the regulating groups RB1 and RB2 as well as the shutdown groups SB3 and SB4.

The thermal power of the core was 160 MW. The inlet mass flow was fixed to 1924 kg/s/assembly and the inlet temperature was set to 566.5 K (560 °F from BEAVRS). Outlet pressure was set to 12.76 MPa (1850 psi from BEAVRS).

The nodal model used one node per assembly with 40 axial nodes in the active core, 8 in the bottom reflector and 12 in the top reflector. The node heights were variable in order to capture the axial variation in the materials. The radial reflector was modeled with one assembly pitch thickness.

The thermal hydraulics solver modeled each assembly as a separate channel. The fuel behavior solver modeled a single representative fuel rod per assembly. The axial nodalization of the thermal hydraulics and fuel behavior solvers equaled that of the nodal neutronics solver.

3.2. Evaluated Parameters

The aim in this article was to evaluate the instantaneous control rod group worths in different conditions (CZP, HZP, HFP), evaluate the fulfillment of the shutdown margin required for short and long term shutdown and evaluate various reactivity coefficients for the core at power levels between 0 % and 100 %. All simulations were conducted for the fresh core.

4. MODELING APPROACH

4.1. Group Constant Generation

Serpent was used to generate homogenized group constants for Ants including both the fuel assembly and the reflector region nodes in the Ants model.

4.1.1. Fuel assemblies

Two sets of fuel assembly group constants were generated, namely the cold zero power (CZP) group constants and the combined hot full power/hot zero power (HFP/HZP) group constants. Equilibrium xenon concentrations were used in the generation of the HFP/HZP set of group constants in order to produce the constants required for xenon calculations in the nodal code.

Group constants were generated for each assembly type in the presence of three different grid options (Zircaloy grid, Inconel grid, no grid) and with each possible control rod segment (AIC, B4C, no rods).

The group constants for fuel assemblies were generated using the fundamental mode critical spectrum method for leakage correction with cumulative migration method [9] based diffusion coefficients.

4.1.2. Reflector regions

The radial reflector region was homogenized using a 2D full core model. Special care was taken in evaluating the diffusion coefficients in the reflector nodes and the discontinuity factors at the core reflector boundary. The method applied in the calculation of these discontinuity factors was based on the process described in [10].

The bottom and top reflectors were homogenized using a 3D assembly model with radially reflective boundary conditions.

4.2. Coupled Calculations

All codes coupled in the Kraken framework need to provide certain functionalities such as accepting and providing data for the coupled *fields*. Each field consists of a vector of numerical data that has an associated *mesh* describing the spatial distribution of the data. The framework currently supports regular and irregular cartesian meshes, regular hexagonal meshes of several types and cylindrical meshes. The meshes can also be nested inside of each other.

The solvers may also provide and/or accept data for a self-chosen set of *variables* that may represent, e.g. heights of control groups, global boron concentration or control variables such as critical boron or equilibrium xenon calculation mode. These variables can be interacted with via the multi-physics driver Cerberus providing a capability to e.g. switch from equilibrium xenon calculation to fixed xenon distributions or to insert or retract specific control groups or control rod assemblies.

The Cerberus input contains solver definitions, input definitions and an user written coupled calculation sequence constructed from basic blocks such as field transfers, solver executions, modifications of solver input variables, iteration loops and convergence checks.

When Cerberus is executed, it will initialize the solver modules and establish socket based communications separately with each solver. Cerberus will then go through the user specified coupled calculation sequence handling the general solution flow as well as the data flow between the solvers. The field and variable data obtained from the solvers as well as that sent to the solvers is written to files for post-processing purposes.

5. SIMULATIONS

5.1. Evaluation of Control Group Worths

The control group worths can be evaluated for several power levels at various insertions using a single Cerberus input by defining iteration loops in the input. The outer loop iterates through various power levels and starts with the iteration of the critical reactor state for the specified power level including all core physics solvers and the iteration of critical boron and equilibrium xenon. Once

the critical state is found, the boron and xenon concentrations can be fixed and the control groups are then evaluated separately using iteration loops with the group insertion changing on each iteration and only the neutronics solution being updated. All field transfers and control variable updates (control rod movements, xenon and boron iteration etc.) are handled by the multi-physics driver based on the Cerberus input.

Table 1: Control group worths coefficients evaluated for the SMR core at different conditions (pcm). The one sigma statistical uncertainty for the Serpent results is 4 pcm.

	CZP			HZP			HFP		
	Ants	Serpent	A-S	Ants	Serpent	A-S	Ants	Serpent	A-S
RB1	861	874	-13	1974	2012	-38	2084	2221	-137
RB2	2094	2092	+2	2218	2161	-57	2290	2285	+5
SB3	2592	2597	-5	3547	3559	-12	3612	3697	-85
SB4	2592	2596	-4	3547	3560	-13	3612	3703	-91

The control group total worths were evaluated with both calculation sequences at CZP, HZP and HFP. The boron concentration for CZP was 1500 ppm. For HZP and HFP the critical HFP boron concentration evaluated by the reduced order sequence (1061.5 ppm) was used. The Serpent HFP evaluation was conducted with thermal hydraulic fields taken from the reduced order sequence. The results are shown in Tbl. 1. A very good agreement can be seen in CZP, whereas slightly larger differences can be observed for the regulating groups in HZP conditions. In HFP conditions, the differences increase further for three of the groups.

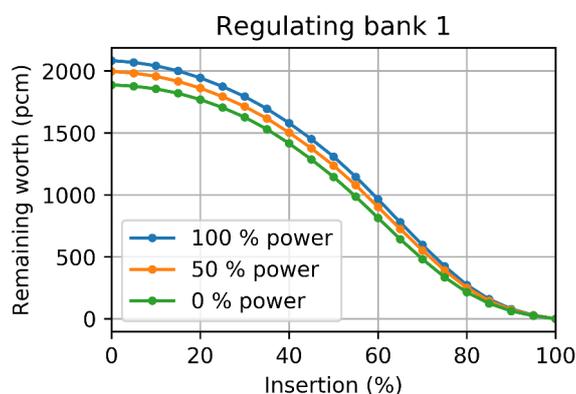


Figure 2: Available worth of regulating group 1 as a function of group insertion.

The group worths were also evaluated at different levels of insertion and reactor power using the reduced order calculation sequence. Fig. 2 shows the results for regulating group 1, situated in the central region of the core. Its worth has a clear dependence on the reactor power.

5.2. Evaluation of Shutdown Margin

The different components of the long term shutdown margin were evaluated using the reduced order sequence and are collected in Tbl. 2. Considering the hot shutdown of an operating reactor at hot full power (HFP) using control rods, the total available control rod worth needs to account for multiple phenomena. During normal operation, the regulating groups may be partly inserted to the core up to the power dependent insertion limits (PDIL), the margin needs to also cover the single failure of the highest worth control rod assembly (CRA) being stuck out, finally in order to

Table 2: Shutdown margin for the SMR core. Evaluated at HFP critical boron.

Parameter	(pcm)
1. Total available CRA worth at HFP	18187
2. Effect of power dependent insertion limits at HFP	332
3. Highest worth CRA stuck out	5317
4. Power defect	662
5. Long term cooling	924
6. Xenon worth	2353
7. Net margin for hot shutdown (1. – 2. – 3. – 4.)	11876
8. Net margin for long term shutdown (7.–5.–6.)	8599

prevent recriticality due to cooling to hot zero power (HZZP) conditions, the power defect due to fuel and coolant temperature difference between HFP and HZZP needs to be also covered.

If further considering the long term shutdown to cold zero power (CZZP) conditions the additional cooling of the core needs to be accounted for as does the eventual decay of ^{135}Xe in the core. The approach taken here for evaluating the shutdown margin is similar to that taken in the NuScale licensing documents [7].

The shutdown margin evaluation utilized several capabilities of Kraken:

- Movement of control rods in the neutronics model (worth evaluations, effect of PDIL).
- Modification of the thermal hydraulic fields passed to the neutronics solver (power defect, long term cooling).
- Modification of the xenon field used by the neutronics solver (xenon worth).

The net margin for hot shutdown was approximately 11.9 % and for long term shutdown approximately 8.6 %.

5.3. Evaluation of Reactivity Coefficients

The multi-physics driver supports modifying the coupled fields via simple arithmetic operations (+, -, ×, ÷) which can be utilized in the calculation of reactivity coefficients.

For example, the fuel temperature (Doppler) and moderator temperature spectral coefficients can be evaluated by simply adding a small temperature value (e.g. +5 K) to the corresponding field and calculating the change in system reactivity. The moderator density (void) reactivity coefficient can be evaluated by decreasing the moderator density by a small percentage (e.g. ×0.99) whereas the power coefficient can be obtained by increasing the total power by a small margin (e.g. ×1.01) and re-converging between the different coupled solvers. The boron reactivity coefficient can be calculated through a small addition to the boron concentration (e.g. +1 ppm).

The combined moderator temperature and density coefficient requires a more specialized approach as the modified moderator density needs to correspond to the modified moderator temperature,

Table 3: Reactivity coefficients evaluated for the SMR core at HFP conditions (all rods out). One sigma statistical uncertainties given for the Monte Carlo results.

	Ants	Serpent <i>Ants fields</i>	Serpent <i>Serpent fields</i>
Fuel T (Doppler)	-2.53 pcm/K	-2.50 ± 0.07 pcm/K	-2.78 ± 0.07 pcm/K
Moderator T (spectral)	N/A	-2.10 ± 0.18 pcm/K	-3.03 ± 0.18 pcm/K
Moderator T, ρ	-24.1 pcm/K	-18.3 ± 0.36 pcm/K	-27.19 ± 0.46 pcm/K
Void	-51.5 pcm/%	-45.2 ± 3.6 pcm/%	-64.2 ± 3.7 pcm/%
Power	-12.2 pcm/%	-7.21 ± 0.72 pcm/%	-3.55 ± 0.74 pcm/%
Boron	-17.1 pcm/ppm	-10.2 ± 0.72 pcm/ppm	-13.1 ± 0.74 pcm/ppm

which requires a steam table lookup. At the moment, such a routine has not been implemented and for these calculations the modified density field was written to a file using an ad-hoc Python script and used to set the value of the moderator density field in the multi-physics driver.

Evaluating the reactivity coefficients at different power levels is rather straightforward since the neutronics power can be adjusted via the multi-physics driver in a manner similar to that used with the control group worth evaluations.

Tbl. 3 shows the evaluated reactivity coefficients for the SMR core. As the legacy group constant model used with Ants in this work does not contain independent parametrization for coolant temperature and density, the moderator spectral coefficient was not evaluated. Serpent was used to separately evaluate the reactivity coefficients using the converged TH fields from the reduced order and the high-fidelity sequences. The Doppler coefficient is well predicted by the reduced order sequence whereas larger differences can be seen in the moderator temperature and density reactivity coefficients. The power and boron reactivity coefficients seem to be overpredicted by the reduced order sequence in this case. The results in general indicate that the legacy group constant model should be replaced with a more modern one in the short term.

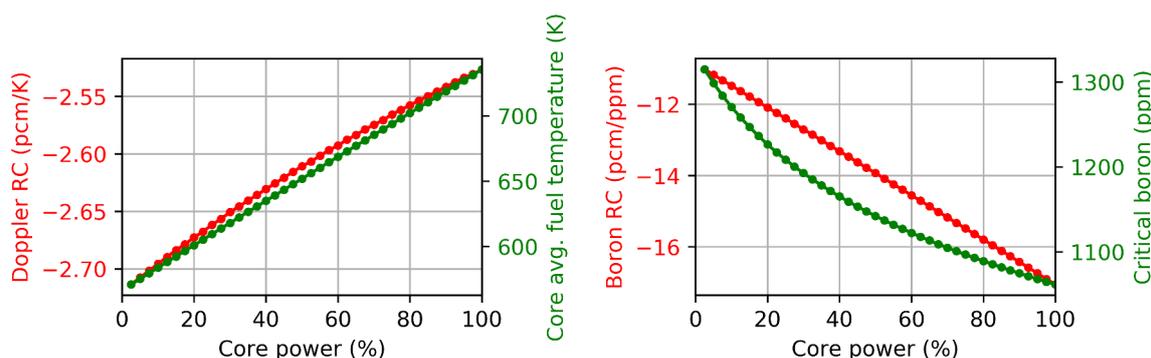


Figure 3: Fuel temperature and boron reactivity coefficients evaluated with the reduced order calculation sequence at various power levels.

Fig. 3 shows the fuel temperature and boron reactivity coefficients evaluated with the reduced order calculation sequence as a function of reactor power. As the fuel temperature increases along increasing core power, the reactivity effect from an additional increase in fuel temperature is reduced. On the other hand, at higher core powers the critical boron concentration is reduced and the reactivity effect from a one ppm boron addition is magnified.

6. CONCLUSIONS

The simulations demonstrated the capability of the Kraken computational framework to evaluate not only the converged steady state multi-physics solution for a realistic reactor core geometry but to also execute point perturbations required for the evaluation of control rod worths, shutdown margins and reactivity coefficients. This capability is an essential requirement in order to apply the framework to licensing relevant safety evaluations. The nodal diffusion and Monte Carlo based calculation sequences produce results that compare to each other in a reasonable manner. The actual validation of the sequences will be started with fresh core calculations of the BEAVRS benchmark [8].

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