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Development of Coupled Neutronics and Fuel Performance Analysis Capabilities between Serpent and TRANSURANUS

Heikki Suikkanen[a,*], Ville Rintala[a], Arndt Schubert[b], Paul Van Uffelen[b]

[a]*Nuclear Engineering, LUT School of Energy Systems, LUT University, P. O. Box 20, FI-53851 Lappeenranta, Finland*
[b]*European Commission, Joint Research Centre (JRC), Karlsruhe, Germany*

Abstract

Monte Carlo reactor physics code Serpent is coupled with the fuel performance code TRANSURANUS for steady state analyses including fuel depletion calculations. A two-way coupling is developed, such that the codes exchange data with each other and the solution is obtained as the result of iterations between the two codes. The coupling scheme is external, based on data exchange via output files, such that no source-level modifications are needed on either of the coupled codes. A separate driver program is written to run the coupled calculation including exchange of data, monitoring and determination of convergence. Data provided by the fuel performance code includes the radial temperature distribution and the radius changes in the axial slices of a fuel pin while the reactor physics code provides the linear power and fast neutron flux along with the form of the radial power density in the corresponding axial slices of the pin. The coupling is demonstrated in a calculation case based on a fuel performance benchmark for a burnable absorber rod with gadolinium. The results compared with stand-alone fuel performance calculations demonstrate the capabilities of the coupled calculation system to enhance fuel performance analyses via higher-fidelity neutronic solver capable of providing an accurate neutron flux solution for the rod of interest.

Keywords: reactor physics, thermo-mechanics, coupled calculation, Monte Carlo neutronics, burnup calculation, fuel behaviour

*Corresponding author
Email address: heikki.suikkanen@lut.fi (Heikki Suikkanen)

1. Introduction

A multitude of physicochemical processes working at different spatial and temporal scales take place in a nuclear reactor. Core neutronics and fuel burnup consider the nuclear reactions mainly induced by neutrons, either directly or indirectly, resulting in changes of the fuel isotopic composition. Core thermal-hydraulics governs the flow of coolant fluid as well as the transfer of heat in the core, while the fuel thermomechanics considers also the deformations in the fuel and the cladding, and in a wider scope of fuel behaviour or performance analyses take into account several physical and chemical phenomena occurring in a fuel pin. These all are heavily interdependent of each other, and thus, computer codes applied for reactor design, operation and safety analyses aiming to accurately predict the behaviour of a reactor need to account for the relevant feedbacks between the various processes. Although such computer codes have already been developed and used for decades, the evolution of computer hardware makes it feasible to utilise computationally expensive calculation approaches based on less approximations and more on first principles for best-estimate analyses at an increasingly larger scale and for more industry-like applications (Ferraro et al., 2019), even considering couplings between the multiple physics.

Development and improvement of such analysis capabilities is constantly ongoing in several projects ranging from large efforts that can involve multiple countries or organisations, such as the development of the European NURESIM platform (Chauliac et al., 2011), the MOOSE simulation environment at the Idaho National Laboratory (Gaston et al., 2009) or the work within the CASL consortium established by the US Department of Energy (Turinsky and Kothe, 2016), to more modest, yet still very useful contributions by individual organisations or research groups. Examples of such recent contributions related especially to coupling neutronics with fuel performance codes include the development of a coupling between the fuel performance code TRANSURANUS and the reactor dynamics code DYN3D (Holt et al., 2015) as well as the coupling of Serpent with the fuel performance codes ENIGMA and Finix (Valtavirta et al., 2017). It should be noted that the couplings developed between similar or even

same codes by different groups can still differ from each other significantly in the way they have been implemented and in what data is actually transferred between the codes.

Following a similar path as the latter mentioned couplings between separate solvers, we develop a coupling between the Monte Carlo reactor physics code Serpent 2 (Leppänen et al., 2015) and the fuel performance code TRANSURANUS (Lassmann, 1992). The purpose at this point is not to develop a comprehensive multiphysics toolset, such as MOOSE or NURESIM, but a lightweight tool specifically to enhance fuel performance analyses. The coupling is realised by means of a separate driver program that is written to execute the two codes and control the coupled solution process. This approach is considered, first of all, to be user friendly as it essentially requires no modifications to the source, no special versions of either of the coupled codes nor installation of additional libraries or frameworks, thus making it straightforward to deploy into use.

The motivation for coupling the two codes is twofold. First, to improve the results of the fuel performance calculations by utilising the power distributions resulting from a neutron transport calculation by Serpent. Second, to enhance the results of the reactor physics calculations by utilising the fuel pin temperature distributions provided by TRANSURANUS in place of some, more or less representative, constant temperature approximations. Although TRANSURANUS comes with in-built models for the rod radial power distribution, replacing them with an actual neutron transport solver is expected to improve the predictions especially in cases where the neutron diffusion approximation proves insufficient, for example, in the presence of burnable absorbers, such as gadolinium. A Serpent calculation model can consist of at least the fuel assembly where the fuel pin of interest is located but in addition, it can include additional neighbouring fuel bundles and structures, such as control rods or assemblies to obtain a more accurate flux distribution for the rod of interest. This is something that the internal neutronic models of fuel performance codes are not capable to account for by themselves as such codes only consider a single rod of interest. TRANSURANUS, in turn, provides Serpent the rod temperature distribution so that the temperature effect on the cross sections can be accounted for in the neutronics calculation, which further affects the power distribution. The final solution is obtained as the result of iterations between the two solvers. There is no core thermal hydraulic solver included in the

coupled calculation scheme at the current stage, so representative thermal hydraulic boundary conditions for the fuel performance solver and the coolant conditions for the neutronics solver need to be provided based on external thermal hydraulic calculations. Thus, the core thermal hydraulics are treated essentially in the same way as would be done in stand-alone fuel performance or neutronic calculations.

In this paper, the focus is on improving the fuel performance results and the structure of the paper is as follows. A description of the coupled calculation system is given in Section 2. The coupled calculation system is also illustrated with an example calculation adapted from a fuel performance benchmark with rods containing gadolinium as burnable absorber. Along with a description of the demonstration calculation, specific attention is given in Section 3 to the extraction of radial power distributions from the Serpent results and the convergence of both, the actual coupled solution process between the neutronics and fuel thermo-mechanics, but also the radial power distributions obtained from Serpent via bin-based tallies. The results along with comparisons to stand-alone calculations with TRANSURANUS, are presented in Section 4. Finally, conclusions are drawn in Section 5 along with a brief overview of the perspectives for the coupled scheme.

2. Description of the Coupled Calculation System

Serpent and TRANSURANUS are coupled externally in the sense that they are not linked together at the source code level. In fact, there are no source code level modifications needed in either of the two codes as contrary to memory based data transfer, the coupling makes use of the already existing data input and output routines so that the data exchange is handled via ASCII files the codes read and write. This way there is no need to maintain the specific coupled calculation functionalities in either of the codes. The coupling provides an actual two-way data transfer meaning that the codes are executed sequentially and provide input for each other in between the runs. This iterative process continues until predefined criteria are reached, and thus, a converged solution of the current state point, such as a burnup step, is obtained. This approach, utilising Picard iteration technique, is well suited for coupling existing solvers to result

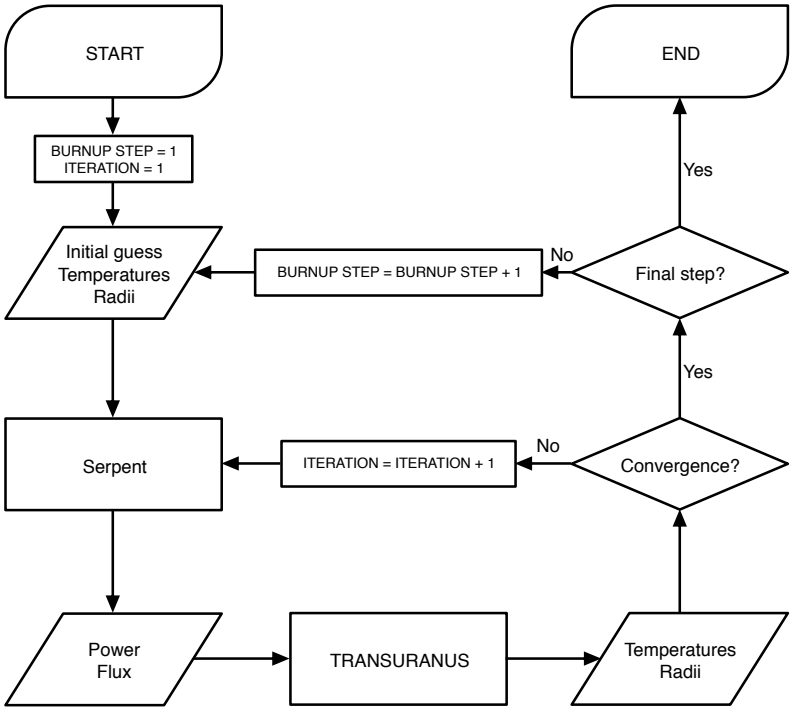

Figure 1: Flowchart of a coupled Serpent - TRANSURANUS calculation.

in a tightly coupled solution as discussed in more detail, for example, by Mahadevan et al. (2014) along with other coupling strategies. Data that TRANSURANUS provides for Serpent includes the radial temperature and strain distributions in axial slices, while Serpent provides TRANSURANUS with the power distribution in the fuel in the form of linear powers and radial form factors, and the fast neutron flux (> 1 MeV) axial distribution in the cladding. Solution convergence is monitored by an external driver program that also controls the whole coupled calculation system and executes the two codes in sequence. The general flowchart of the coupled calculation process is shown in Figure 1.

Currently, the coupling can be used for steady state analyses, including burnup cal-

culations performed as a series of steady state calculations. Serpent is equipped with advanced burnup calculation capabilities, such as the Chebyshev Rational Approximation Method (CRAM), capable of solving accurately and efficiently large burnup matrices, typically including 1200-1600 nuclides in the calculation (Pusa and Leppänen, 2013). However, no nuclide data is currently transferred from Serpent to TRANSURANUS as both codes perform independent burnup calculations. In TRANSURANUS this is handled by the TUBRNP subroutine which considers only the few most relevant actinides and fission products. However, in the coupled calculation TRANSURANUS uses the power distributions affected by the more detailed nuclide inventory solution as calculated by Serpent.

TRANSURANUS requires thermal hydraulic boundary conditions, such as coolant pressure and either the cladding outer temperature or the coolant temperature and the heat transfer coefficient. Coolant conditions are also important for the neutronics calculations by Serpent. These need to be provided for the two codes as no core thermal hydraulic solver is currently included in the coupled calculation system. Representative boundary conditions can be obtained in the same way as they would be obtained in stand-alone fuel performance or neutronic calculations, that is, from external calculations with a suitable thermal hydraulic solver. Moreover, in case of fuel performance benchmarks, such as utilised in the demonstration calculation of this work, it is typical that the thermal hydraulic boundary conditions based on the reactor operation history are pre-calculated and provided in the benchmark description.

2.1. Overview of Serpent

Serpent is a three-dimensional continuous-energy Monte Carlo reactor physics and burnup calculation code developed at VTT in Finland since 2004 with contributions by the active international user community (Leppänen et al., 2015). In addition to being well capable of handling traditional reactor physics applications, such as criticality and spatial homogenisation calculations, the current version, Serpent 2, has been developed towards becoming a multi-purpose tool also covering photon transport and being applicable in research fields like fusion energy and medical physics. Most relevantly for the work in this paper, Serpent 2 has been implemented with versatile capabilities

facilitating coupling with external codes for high-fidelity multi-physics simulations.

2.1.1. Multi-Physics Interface

Serpent 2 has a universal multi-physics interface that simplifies coupling it with external codes that exchange material temperature and density fields to the power distributions provided by Serpent (Valtavirta, 2017). The multi-physics interface comes with several interface types intended for different purposes; the interface types 5 and 6 being designed for coupling Serpent with traditional fuel performance codes.

In practice, coupling Serpent with a fuel performance code requires a separate interface file in addition to the regular input file defining the geometry, material isotopic compositions, run parameters, etc. The separate interface file lists the fuel pins for which data is to be exchanged and defines the spatial bins used for scoring fission events and neutron flux. It also provides temperatures at specific coordinate points, which virtually update the Serpent geometry model as calculated by the fuel performance code (i.e. changes in the fuel pin radii are taken into account in neutronics calculations). After a successful neutron transport calculation, Serpent writes a separate output file with the power and neutron flux data for the bins defined in the interface file.

2.1.2. Obtaining Radial Power Distributions

Serpent, being a Monte Carlo reactor physics code, tracks individual neutrons as they traverse in a medium and experience events based on probabilities dictated by the material cross sections. Depending on whether analog or implicit estimators are used, these events can either be actually occurring ones (analog) or represent the expected frequency of a particular event (implicit) via collision or track-length based flux estimators (Leppänen, 2007). Events are scored in domains or bins that can cover, for example, different spatial regions or neutron energies. Thus, extracting the fission power distribution in a fuel rod can be done by dividing the rod into spatial bins and scoring, in each of the bins, the fission events multiplied by the heat deposition associated with the particular nuclides. The number of the bins can be increased for increased resolution but this will also require increasing the number of neutron histories in the Monte

Carlo simulation to obtain sufficient statistics for the smaller bins, thus increasing the computational effort. Using too few bins (i.e., low resolution), on the other hand, can result in averaging out important details of the distribution.

The power and its radial distribution in the axial slices of a fuel rod are the main data that Serpent provides for the fuel performance code in a coupled calculation. It needs to be ensured that the bin mesh in a rod has the resolution to resolve the form of the distribution with the desired accuracy and also that sufficient statistics are obtained for the bins (i.e., enough events are scored) so that the power distribution has properly converged. An example for a fuel rod with gadolinium as the burnable absorber is shown in Figure 2 where the radial resolution of the bin mesh or the number of simulated neutron histories is varied. The axial thickness of the bins in each case is kept constant and is 10 cm while the total length of the rod is 100 cm. It can be seen that using a too coarse bin division will, for example, seriously underestimate (average out) the maximum power density at the rim, while using an insufficient number of simulated neutron histories results in a high statistical variance in the bins and will not produce a smooth distribution.

It is intuitive to divide the rod cross-section into rings of equal area as also done in the cases shown in Figure 2. This naturally leads to an increased resolution in the radial direction towards the rim. This is beneficial not only because of the equi-volume bins obtained for scoring events, but as the power distribution typically has a steep gradient at the rim region due to the formation of fissile plutonium isotopes with burnup or when the fuel contains burnable absorber that burns out in layers from the rim towards the centre. This is also the division method implemented in Serpent for both obtaining radial power distributions through the multi-physics interface and defining burnup regions. For these reasons, this approach is used to construct the bins for retrieving radial power distributions. However, as can be seen in Figure 2, the bin-based methodology produces distributions with a staircase form; an undesired effect, which can be diminished by increasing the radial resolution of the bin mesh. In practice it is not possible to increase the number of the bins excessively due to the escalation of the computational effort as already discussed above. This is especially true for a coupled calculation where the neutron transport calculation for a single state point is performed

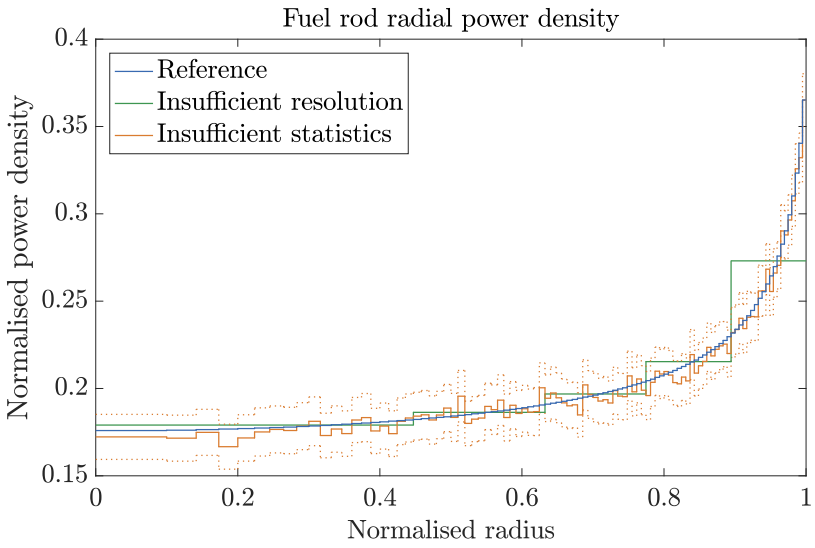

Figure 2: Radial power density distribution in a 10 cm axial slice of a rod with the total active height of 100 cm. Profiles obtained with only 5 bins of equal volume (green) and with 100 bins but too few simulated neutron histories (orange, also showing the 3σ confidence intervals with dotted line) compared to a high resolution (100 bins) reference solution obtained with 10^{11} simulated neutron histories. The error bars of the reference and the coarse resolution bins are not plotted as they would not be distinguishable from the mean values.

multiple times.

A methodology illustrated in Figure 3 is developed to smooth out the power distribution obtained from Serpent before transferring it to the fuel performance code. This methodology is, basically, a linear interpolation based on connecting the midpoints of the bin power histograms with line segments when they are plotted as a function of radius. In addition, the value at the rod boundary is approximated by extrapolating the last line segment to the outer boundary; an approximation that still underestimates the actual maximum value at the boundary if the bin resolution near the boundary is low. Now, the radial power distribution is obtained as a piecewise linear fit which is then renormalised to conserve the total power of the corresponding axial slice. The power distribution is provided to the fuel performance code as values at the locations corresponding to its radial nodalisation. These values are now obtained from the piecewise

linear fit instead of the original histogram profile avoiding providing the fuel performance code a profile with a staircase form.

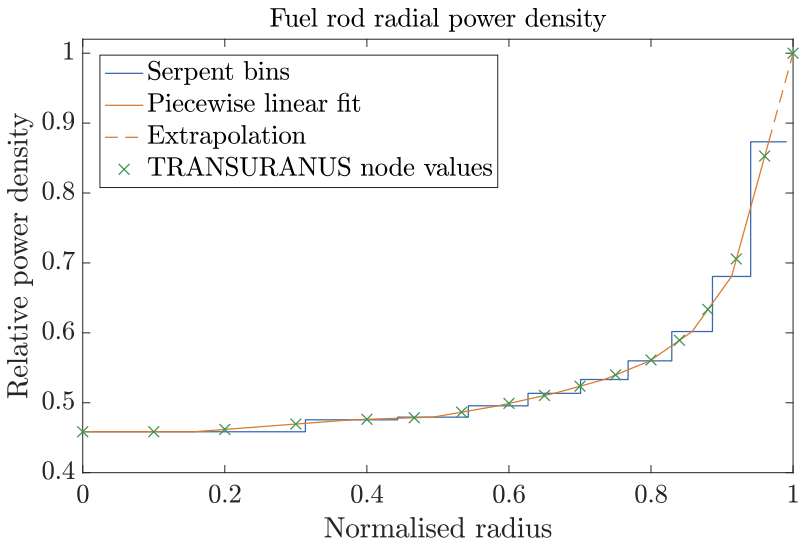

Figure 3: Methodology developed for mapping the radial power distribution to TRANSURANUS that smooths out the staircase form resulting from the bin-based power tallies of Serpent.

Serpent considers currently (in version 2.1.30) that all energy is locally deposited where fissions occur and calculates the deposited energy κ for different fissionable nuclides i based on the fission Q-values as

$$\kappa_i = \frac{Q_i}{Q_{U235}} \kappa_{U235}, \tag{1}$$

where $\kappa_{U235} = 202.27$ eV is the energy deposition for U-235 (Valtavirta, 2017). This is a crude approximation as it assumes that all energy is deposited in the fuel, not considering that part of the heat is also deposited in the cladding coolant and other structures due to neutrons as well as beta and gamma radiation.

2.2. Overview of TRANSURANUS

Fuel performance codes such as TRANSURANUS are typically based on the so called 1.5 dimensional representation of a single fuel rod, for which solution variables

are obtained in radially distributed node points in axially segmented slices. The codes solve the thermo-mechanics of the rod and account for the effects of fuel burnup via models and correlations. Extensive overview of the various models and capabilities is given by Van Uffelen et al. (2019, 2010). As boundary conditions a fuel performance code needs the rod axial power distribution as well as the coolant temperature and pressure. These are typically obtained from external core neutronic and thermal hydraulic calculations utilising available operating data of the particular reactor or experiment. The rod temperature distribution depends on the power distribution and as the temperature distribution affects the mechanical models it is essential to have an accurate power distribution for the rod in the first place. The rod linear power history during an irradiation period is provided for the fuel performance code. This is obtained, for example, from calculations with a core simulator code. A fuel performance code, such as TRANSURANUS, then uses an inbuilt neutron diffusion solver to calculate the radial power distribution in the axial slices of the rod. It is known that the diffusion approximation of the neutron transport equation in the vicinity of strongly absorbing isotopes like ^{155}Gd requires correction. For this purpose, specific burnup dependent correction factors have been developed for specific fuel types by means of deterministic neutron solvers such as HELIOS. In a second step, the data exchange has been considered between such codes and TRANSURANUS as described in Section 2.2.2.

2.2.1. Overview of TUBRNP

For each timestep simulated with a fuel rod code like TRANSURANUS, the power generated per unit length in each axial segment due to fission is prescribed as a boundary condition. The radially averaged power density in each axial segment and timestep modelled is therefore known. Nevertheless, the corresponding radial profiles of the power density within the fuel pellets may deviate significantly from uniformity as irradiation proceeds, and therefore may have a significant effect on the radial temperature distributions in the pellets (Schubert et al., 2008b). These radial distributions are unknown and must be provided as input or calculated using a neutronics model for each axial section. The former approach was the norm until the early 1980s, when neutronics models began to be introduced (Van Uffelen et al., 2019). In the TRANSURANUS

burn-up model (TUBRNP) (Lassmann et al., 1994, 1998) the calculation of the radial power profiles is split into (a) the approximation of the neutron flux through thermal diffusion theory and (b) the computation of the local concentrations of the relevant actinide nuclides that are either fissile or fertile. TUBRNP so far calculates the local concentration of the most abundant nuclides of U, Np, Pu, Am and Cm by solving incrementally the differential nuclide evolution (Bateman) equations, as a function of the radial position across a fuel pellet. These local quantities are required for the determination of the local power density, the local burn-up as well as the local fission products Nd, Xe, Kr, Cs and He. In more recent development work (Tijero Cavia et al., 2018), TUBRNP was extended with nuclides relevant for thorium-containing fuels, i.e. ^{232}Th, ^{233}U and ^{234}U.

2.2.2. Features Facilitating Coupling with External Codes

TRANSURANUS comes with a couple of convenient features that facilitate the coupling with external codes. There is a capability for reading in a radial power distribution calculated by an external code. This is done via a separate input file, called *formfext*, in which the power density form factors in the radial nodes of TRANSURANUS are given. Thus, by updating the *formfext* file before running TRANSURANUS, this feature allows the input of a radial power distribution calculated by an external code. Another convenient feature is the restart run capability. This feature allows saving the calculation state after the final iteration of a state point and then continuing from there when TRANSURANUS is invoked to calculate the next state point in iterations between Serpent.

2.3. External Driver Program

A separate driver program is written in the Perl programming language to control the coupled calculation process between Serpent and TRANSURANUS. It runs the two codes sequentially, monitors convergence and exchanges data in a correct format between the coupled codes. The driver program saves the input and output data for which it maintains an organised directory structure.

2.3.1. Transferring Data

Serpent performs the neutron transport calculation by the Monte Carlo method and as the result, provides the power and the fast neutron flux distributions in the fuel rods. The multi-physics interface of Serpent is used for data input and output. The driver program processes the output provided by the Serpent multi-physics interface into the format that TRANSURANUS can read as an input. Data is provided to TRANSURANUS via two files. The axial distribution of the rod linear power and fast flux is given for each axial slice in the main input file. Radial power distribution is provided through the separate *formfext* file containing the power density form factors in the radial nodes of each axial slice.

TRANSURANUS performs the thermo-mechanical calculation of a single fuel rod. It provides Serpent the temperatures in the radial nodes of each slice and the coordinates of these nodes. The data is extracted from the binary output file of TRANSURANUS using the separate post-processing tool TuPlot that comes bundled with TRANSURANUS. The driver program again processes the resulting text file with node coordinates and temperatures into the format that Serpent can read in via the multi-physics interface.

2.3.2. Executing Coupled Codes

Serpent is run in the coupled calculation mode, that is, utilising the multi-physics interface, so that after finishing the calculation of a single iteration it will go to sleep mode and wait for a signal to proceed after TRANSURANUS has finished and the driver program has updated the interface file.

After Serpent has finished its part of the current iteration step, the driver program forms updated input files for each fuel rod participating in the coupled calculation and initiates a TRANSURANUS calculation for each rod. The separate TRANSURANUS runs are currently not parallelised but executed in sequence. Solving the separate rods in parallel would naturally reduce the time for the fuel thermo-mechanics part of the coupled calculation process but as the Monte Carlo neutronics part completely dominates the total solution time, the gain in parallel solving the fuel rods in TRANSURANUS would be rather insignificant. The restart functionality of TRANSURANUS is

utilised to save the final converged burnup step solution for TRANSURANUS to use as a starting point in the next burnup step.

2.3.3. Monitoring Convergence

An especially important task that the driver program handles is the monitoring and determination of convergence between the coupled codes. The convergence criteria used by Serpent in coupled calculation mode as described by Valtavirta et al. (2017) are utilised. However, instead of letting Serpent monitor and determine convergence, the convergence criteria are implemented in the driver program that controls the coupled calculation in this case. Two parameters are defined and solved for both power and temperature fields between subsequent coupled calculation iterations.

Changes between iterations in the power and temperature fields of all coupled fuel rods are monitored during the coupled solution process. The local relative differences between, for example, temperature fields of successive iterations are calculated as

$$\epsilon_i^n = \frac{T_i^n - T_i^{n-1}}{T_i^n}, \tag{2}$$

where n denotes the current iteration value and i is the spatial index (i.e. a radial node in an axial section of a rod).

Two convergence parameters are derived based on the specific norms of the vector ϵ. First, the infinity norm or maximum absolute value

$$\epsilon_{\max}^n = \max_i \left|\epsilon_i^n\right|, \tag{3}$$

is calculated, which is identified at the spatial location where the highest difference between the solution of the subsequent iterations occurs. Second, average of the Euclidean or ℓ^2 -norm

$$\bar{\ell_n^2} = \frac{1}{N}\sqrt{\sum_{i=1}^{N}\left(\epsilon_i^n\right)^2}, \tag{4}$$

is computed, which represents the relative changes in the whole domain.

The $\epsilon_{\max}^n$ and $\bar{\ell_n^2}$ are calculated and monitored by the driver program for both, the temperature and the power distributions. Convergence criteria are set for these parameters and the iteration loop exits after either the parameter values below the criteria or a specified upper limit in the number of iterations have been reached.

3. Demonstration Calculations

The calculation system is demonstrated with a coupled calculation. The calculation case is defined based on a fuel performance benchmark obtained from the OECD NEA databank, more specifically the NEA-1625 IFPE/GAIN dataset (Turnbull, 2002). This case is selected as it consists of data for rods with gadolinium as a burnable absorber.

The GAIN dataset contains fuel performance data for four Gd_2O_3 doped UO_2 rods irradiated in the BR3 reactor within the BelgoNucleaire GAIN project. Two of the rods contained 3 wt-% and the remaining two 7 wt-% of Gd_2O_3. The rods were irradiated for three cycles, in between which one of the rods also underwent overpower transients in the BR2 reactor. Being a fuel performance benchmark, the GAIN data contains very limited reactor physical data making it impossible to build a detailed model in Serpent to reproduce the exact irradiation environment that the rods of interest have experienced. Thus, these calculations should not be considered as a validation but merely a demonstration of the coupled calculation system with a realistic case. The result comparisons to be presented will be between the coupled calculation and stand-alone TRANSURANUS calculations.

3.1. Serpent Calculation Model

The calculation model consists of a single gadolinium-doped rod surrounded by eight fresh UO_2 rods so that a square lattice of 3×3 rods with a pitch of 13.5 mm between the rods is formed. All rods are geometrically identical with fuel pellet diameter of 8.233 mm, rod outer diameter of 9.638 mm and cladding thickness of 0.6105 mm. Each rod has an active length of 100 cm. In addition, above and below of the active length the rods have short zirconium spacer rings and end plugs. The top parts of the rods also have a gas plenum of 6.01 cm. Defined on bottom and on top of the fuel rods there are 20 cm columns of water. Periodic boundary conditions are set for the sides of the rod lattice and black boundary conditions on top and below the rod lattice beyond the water columns. Thus, the calculation geometry represents an axially finite, horizontally infinite array of these 3×3 rod configurations.

The fuel rod with burnable absorber has a density of 10.25 g/cm^3 with 3 wt-% of Gd_2O_3 and the U-235 fraction in the uranium is 3.483 wt-%. The remaining rods

have a density of 10.4 g/cm^3 and consist of UO_2 with the U-235 enrichment of 4.0 %. The cladding and other metallic parts are defined as Zircalloy-4 with the density of 6.56 g/cm^3. The fill gas is helium and the density of the water surrounding the rods is set to 0.779 g/cm^3. JEFF 3.1.1 cross section data are used, including thermal scattering cross sections for water taken at 574 K. The fuel and cladding materials are evaluated at the temperatures obtained from the coupled TRANSURANUS utilising the target motion sampling (TMS) on-the-fly temperature treatment in Serpent (Viitanen, 2015). Water is considered to be at 550 K and the cross sections are adjusted accordingly by utilising the Doppler-broadening preprocessor routine in Serpent.

The burnup calculation is performed with 14th order CRAM and the linear extrapolation time integration method with 10 sub-steps. Based on conclusions from the comparisons between different time integration methods by Isotalo (2013), this time integration method, especially when used with sub-steps, can be a sound alternative to more rigorous but computationally expensive predictor-corrector methods that would basically double the number of neutron transport calculations. Thus, the selected method is considered in the scope of the demonstration calculations in this work to represent a sufficient compromise between accuracy and computing time. Normalisation power and depletion steps are set according to the irradiation history provided in the GAIN benchmark documentation. Thus, the normalisation power is set to the gadolinium rod and updated after each depletion step. The demonstration calculation consists of a total of 15 depletion steps corresponding to 441 days and rod average burnup of roughly 13 MWd/kgU covering the first irradiation cycle of the GAIN rods. This is the most relevant period of time, during which the isotopes ^{155}Gd and ^{157}Gd are burned out. It is acknowledged that the burnup calculation especially with the selected time integration method might require an increased number of short time steps for a highly accurate solution of the nuclide composition. The investigations on the most suitable depletion step lengths and time integration methods are left outside the scope of this work as the current focus is on demonstrating the general functioning of the coupled calculation system and the replacement of the diffusion approximation based radial power distributions in TRANSURANUS with those resulting from a Monte Carlo neutron transport calculation. Although the fuel nuclide composition affects the power

distribution there are also other sources of uncertainties, for example, due to the finite bin resolution of the power tallies and the approximation of the deposition of heat as discussed in Section 2.1.2, which likely have a more pronounced effect on the results.

The active length of each of the rods is divided into 10 sections of equal length for obtaining the linear power distribution. This division corresponds to the axial sections in the TRANSURANUS model. A total of 20 and 10 radial divisions are defined for the central rod with gadolinium and for each of the remaining UO_2 rods, respectively, so that rings of equal area are obtained. Thus, the gadolinium rod consists of 200 and and each of the UO_2 rods of 100 volumetric bins for obtaining power distributions. The same division is used for burnup regions in the rods.

3.2. TRANSURANUS Calculation Model

The TRANSURANUS calculation model of the gadolinium-doped rod of interest is based on the data available in the GAIN dataset essentially with the same dimensions and isotope compositions as described above for the corresponding Serpent model. In the coupled calculation Serpent provides TRANSURANUS the form of the radial power profile, while in the stand-alone TRANSURANUS calculations the rod is defined to contain gadolinium which is taken into account by the TUBRNP subroutine that calculates the radial power distribution and the concentrations of the Gd-155 and Gd-157 isotopes are specified in the input for that purpose. The stand-alone calculations are performed with two different gadolinium models available in TRANSURANUS (see Schubert et al. (2008a) and Ieremenko (2013)). Firstly, the default Gd model (option 1 in the manual) is invoked applying a generic set of effective neutron absorption cross sections that are averaged over burnup, radial position as well as various assembly configurations. Secondly, a configuration-specific set of effective cross sections also depending on burnup and relative radial position is tested. From the options available in TRANSURANUS, the dataset related to a fuel rod with 5 wt-% of Gd_2O_3 and a 3.3 % fraction of U-235 in a VVER fuel assembly (option 102 in the manual) is chosen. This model has been derived from neutron transport calculations for a specific VVER fuel configuration with gadolinium-doped fuel. The model is selected on the basis that from the available options in TRANSURANUS, it best resembles the

configuration of the demonstration calculation.

The correlations generally recommended in the TRANSURANUS manual (JRC, 2015) for material properties are used, including, for example, fuel thermal conductivity model suitable for fuel containing Gd (Schubert et al., 2003). The rod active length is divided into ten axial slices, each 10 cm in length. Radially the fuel region is divided into 5 evenly distributed coarse zones that have internal division to 3, 3, 4, 5 and 6 evenly distributed fine mesh points with the number increasing towards the rim. The cladding has one coarse zone with 10 internal mesh points. No separate mesh refinement study is performed as the purpose at this point is merely to demonstrate the coupled calculation and all result comparisons are performed between cases using identical nodalisation.

During the coupled calculation, Serpent calculates the linear power and the fast neutron flux values for each of the axial slices. The driver program writes these to the time-dependent part of the TRANSURANUS input along with other necessary boundary conditions including the coolant pressure and the axial distribution of the cladding outer temperature, for which values provided in the GAIN dataset are used. The linear power and fast neutron flux distributions obtained as the result of the coupled calculation are also used as input in the stand-alone TRANSURANUS calculations, thus making the direct comparison between the radial power profiles calculated by Serpent and the TUBRNP module of TRANSURANUS valid.

The UO_2 rods surrounding the rod of interest are also calculated in the coupled mode, meaning separate TRANSURANUS calculations for each of them. Separate inputs are thus prepared for these rods, similar to the gadolinium-doped rod but excluding Gd-specific correlations and using a slightly higher U-235 enrichment without gadolinium.

3.3. Convergence of the Radial Power Distributions

As discussed above in Section 2.1.2, obtaining an accurate power distribution requires a sufficient number of simulated neutron histories, which depends on the division of the spatial bins used for scoring fissions. A separate power distribution convergence study is performed with Serpent to determine what the sufficient amount of neutron his-

tories would be in this particular case. The amount of neutron histories to be used each time a neutron transport calculation is performed as a part of the coupled calculation is then selected based on this study.

The calculation of the first burnup step with stand-alone Serpent is repeated using an increasing number of neutron histories ranging from $5 \cdot 10^6$ to 10^{10}. The calculation is done utilising the multi-physics interface so that Serpent provides as a result the power in each individual bin along with the associated statistical error. For each of the variable neutron history cases the mean value of the bin relative statistical errors and the standard deviation of the values are calculated and shown in Figure 4. As can be expected, the statistical error of the bin power estimates as well as its variation between the bins decreases as more neutron histories are simulated.

The amount of simulated neutron histories has a major effect on the total calculation time of the coupled calculation as the neutron transport simulation is performed several times for each burnup step. Thus, the amount of neutron histories to be used will need to be determined based on considering both accuracy and performance. Visual examination of the radial power profiles reveals that with $5 \cdot 10^7$ neutron histories some of the extracted profiles still appear slightly rough due to the insufficient statistics. Increasing the amount to 10^8 results in smoother distributions with only slight improvement gained when further increasing the number of neutron histories to $5 \cdot 10^8$. Based on this study, $2 \cdot 10^8$ neutron histories were selected to be used in the actual coupled calculation in this particular case, corresponding roughly to a mean relative error of 0.2 % in the bin power estimates.

3.4. Coupled Calculation Convergence Criteria

A separate convergence study is performed for the coupled calculation to determine suitable values for the convergence criteria. A coupled calculation of the first burnup step is performed with a large number of iterations to see the behaviour of, first of all, the convergence parameters defined in Section 2.3.3, but also the actual Serpent bin power and TRANSURANUS node temperature values. To this end, the convergence parameters as well as the actual temperature and power values are extracted from the calculation output files after each iteration to find out how they evolve with increasing

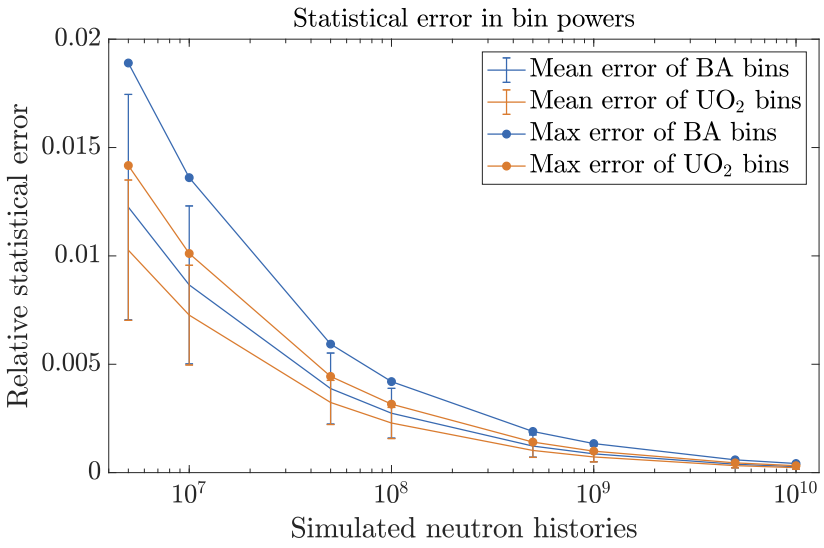

Figure 4: Maximums and means of the relative statistical errors of bin power values obtained in Serpent calculations of a single state point with an increasing number of neutron histories. The 2σ standard deviations associated with the bin mean values are also shown.

number of iterations. These are shown for the convergence parameters in Figure 5 and for the bin powers and node temperatures in Figures 6 and 7, respectively. As can be seen in Figure 5, the convergence parameters come down steeply during the first iterations and then continue to descend more gradually as the number of iterations increase. Similar behaviour can be seen in the power and temperature values in Figures 6 and 7, which show that after roughly 10 iterations the steep change in the bin and node values is over. After this point, further increasing the number of iterations up to 86 only changes, for example, the absolute node temperature values half a degree at most. Thus, the convergence criteria are determined from Figure 5 based on the level of the parameters after roughly 10 iterations, resulting in the infinity norm criterion of 10^{-3} and the Euclidean criterion of 10^{-5}, used for both, power and temperature.

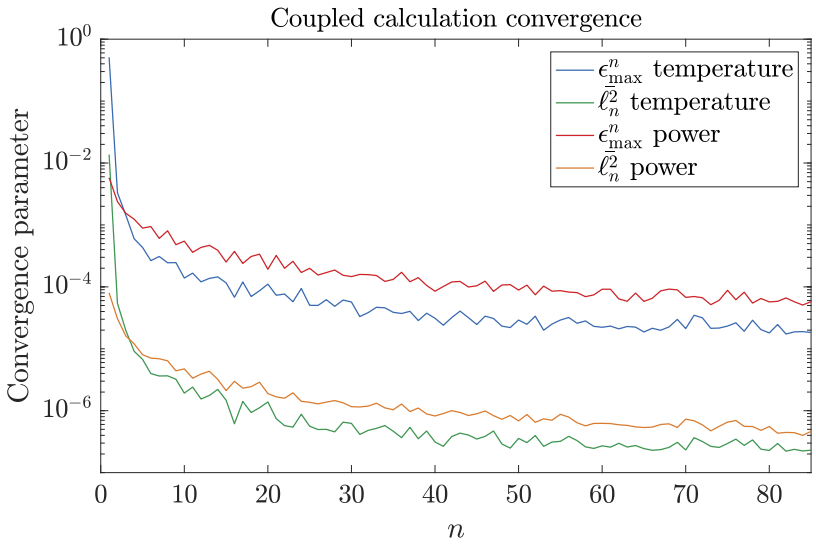

Figure 5: Evolution of the coupled calculation convergence parameters as a function of iterations n.

4. Calculation Results

The coupled calculation was performed using a high-memory calculation node consisting of four Intel Xeon E7-8890 v3 processors with a total of 72 physical cores sharing 2 TB of RAM. The high-memory node is part of a high-performance computing cluster running with the CentOS 7 Linux operating system at LUT University. The coupled calculation consisted of 15 burnup steps, which each consisted from 7 to 10 iterations between the neutronics and thermo-mechanics depending on how quickly the convergence criteria were reached. The calculation took 24.5 days corresponding to 9.7 CPU years.

The total power produced in the gadolinium-doped rod of interest was fixed for each burnup step to the values provided via the power history in the GAIN dataset. These values were used for power normalisation in the Serpent neutron transport calculation. However, the axial and radial distribution of power was obtained as the result of the coupled calculation from the multi-physics output of the final Serpent run of each burnup step. As the axial bin division corresponds to the axial slices used in the TRANSURANUS calculation model, extracting the linear heat rates in the slices is

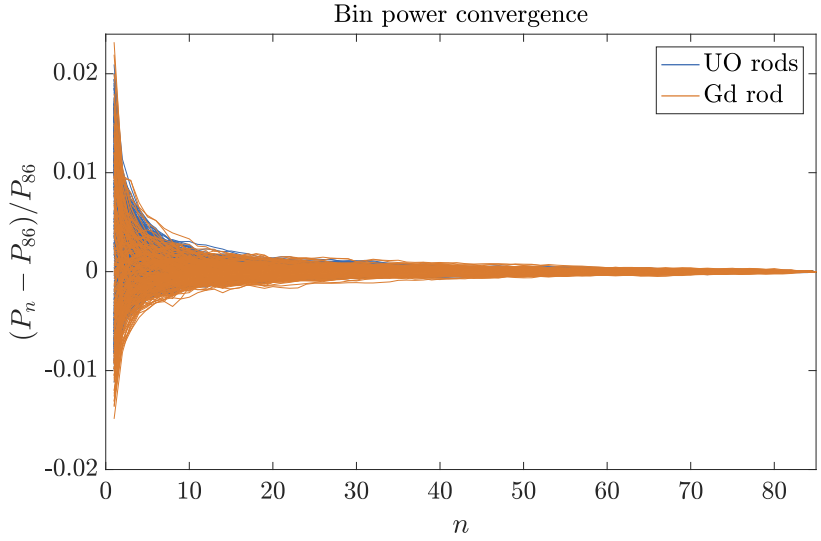

Figure 6: Evolution of Serpent bin powers P during iterations. The iteration number is denoted by n. Results are presented relative to the power value of the last calculated iteration step. Each bin is represented by a separate curve highlighted with a bluish colour for bins belonging to UO_2 rods and with a brownish colour for the bins belonging to the Gd rod.

straightforward. The linear power history obtained in the coupled calculation is shown in Figure 8 for TRANSURANUS slices 2 and 6, located in the bottom and in the middle parts of the rod, respectively. Low power level in the beginning ascending towards the end of the cycle is typical for burnable absorber rods as the concentration of the neutron absorbing isotopes decreases during the irradiation. It should be noted that these exact linear power histories were then also used as input in the stand-alone TRANSURANUS calculations and thus the linear powers in the comparison cases to follow are identical to the ones in the coupled calculation.

Fuel central temperatures during the irradiation period corresponding to the linear power histories in Figure 8 for the bottom and mid part slices are shown in Figure 9. Results are shown for the coupled calculation and for stand-alone TRANSURANUS calculations performed using the default Gd model (option 1) as well as a configuration-specific Gd model (option 102) based on tabulated effective cross section datasets. The default Gd model drastically underestimates the temperature during the

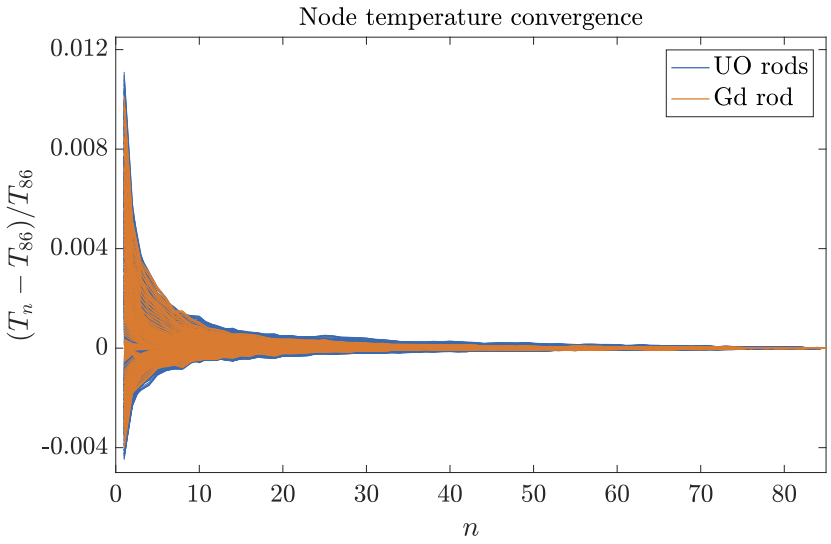

Figure 7: Evolution of TRANSURANUS node temperatures T during iterations. The iteration number is denoted by n. Results are presented relative to the temperature value of the last calculated iteration step. Each node is represented by a separate curve highlighted with a bluish colour for nodes belonging to UO_2 rods and with a brownish colour for the nodes belonging to the Gd rod.

first stages of the irradiation which is well known also from previous work. At the later stages of the irradiation, when most of the neutron absorbing Gd isotopes have depleted, the difference between the default Gd model and the coupled calculation diminishes. The other tested Gd model, although being a configuration-specific model only approximately related to the configuration of the GAIN experiment, predicts temperatures much closer to those obtained in the coupled calculation also during the first stages of the irradiation.

The coupled and the stand-alone TRANSURANUS calculations use identical linear powers in each of the axial slices, the only difference between the cases being the radial form of the power. Thus, the radial distribution of power greatly affects the fuel central temperature. In the coupled calculation, the radial power profile is obtained from the neutronics solution calculated by Serpent accounting also for the rod radial temperature distribution in the evaluation of the cross sections. In the stand-alone calculations, TRANSURANUS estimates the radial profile with its TUBRNP module. This estima-

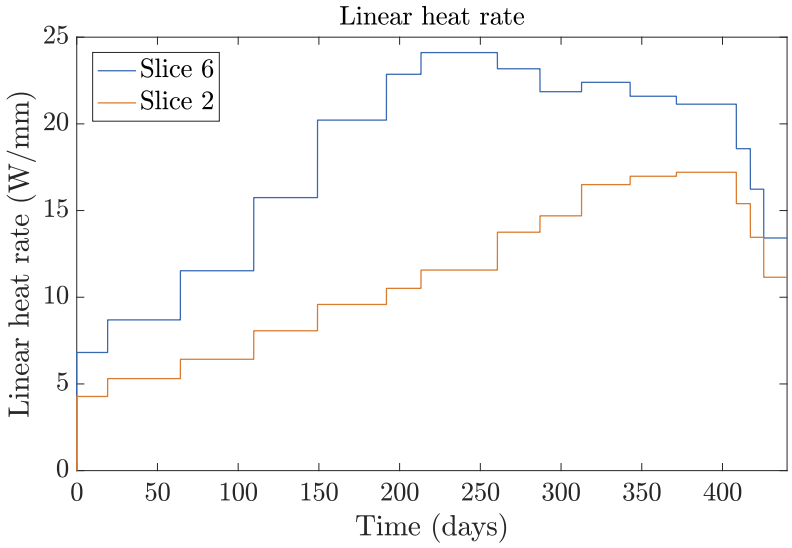

Figure 8: Linear heat rates obtained as a result of the coupled calculation for the bottom (Slice 2) and middle (Slice 6) parts of the rod.

tion or update of radial power profiles is carried out also at intermediate time steps, created by the TRANSURANUS code in the stand-alone calculation, whereas the coupled calculation only updates them at time steps defined by the user in the input file of the coupled system. The effect on the evolution of the central temperature shown in Figure 9 is therefore more pronounced at beginning of irradiation (approximately 250 days) with increasing power, whereas the effect becomes negligible once the Gd isotopes are burned out. Figure 10 shows the radial power density distributions and Figure 11 the corresponding radial temperature profiles extracted from the middle part of the rod (slice 6) at three different burnups extracted from TRANSURANUS output. As can be seen in Figure 10 the default Gd model produces a significantly different form for the power distribution than obtained in the coupled calculation. This is due to the fact that the profile in the coupled calculation results from the Monte Carlo neutron transport calculation, inherently capable of accounting for the full energy dependency available in the used nuclear data library for the cross sections, the strong spatial self-shielding effects of the gadolinium isotopes ^{155}Gd and ^{157}Gd and the pin surroundings

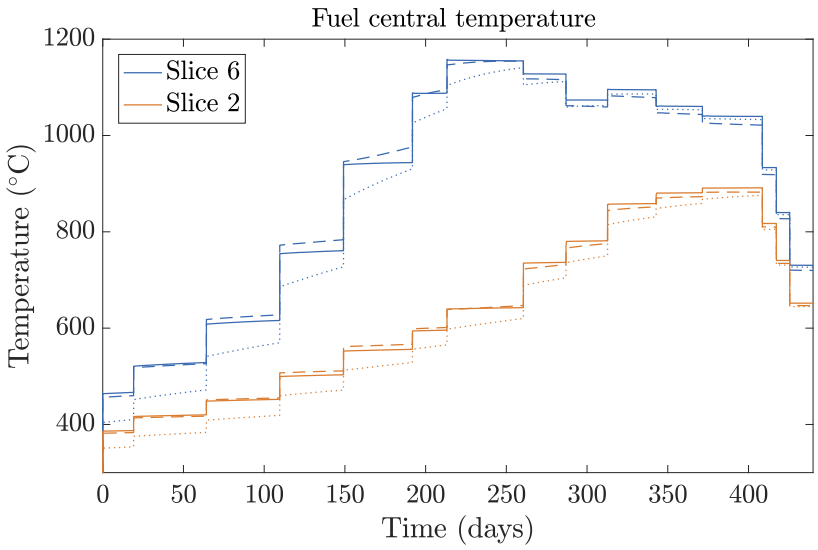

Figure 9: Fuel rod central temperatures during the irradiation period in bottom (Slice 2) and middle (Slice 6) parts of the rod. Coupled calculation results are plotted with solid lines, standalone TRANSURANUS calculation results obtained with the default Gd model (option 1) with dotted lines and with a configuration-specific Gd model (option 102) with dashed lines.

(i.e., water and the neighbour fuel pins), whereas the internal solution of TRANSURANUS has no awareness of the pin surroundings and solves the radial power profile based on the neutron diffusion equation utilising an effective absorption cross section fitted based on experimental data (the default model) or with additional radial dependence based on fitting the model coefficients to neutron transport solutions for specific fuel configurations (the configuration-specific model). The effect on the radial temperature distribution is also significant, although the temperatures during the first stages of the irradiation period are relatively low in the Gd-doped fuel pin. In comparison, the selected configuration-specific Gd model performs significantly better; the power profiles are generally at the same level with those obtained in the coupled calculation with a slight tilt between the profiles leading to either under or over prediction in the centre part of the pin and subsequent over or under prediction at the rim.

As the comparisons in Figures 10 and 11 were only for a single slice, the differences in each of the rod node points between the coupled and the stand-alone calculation with

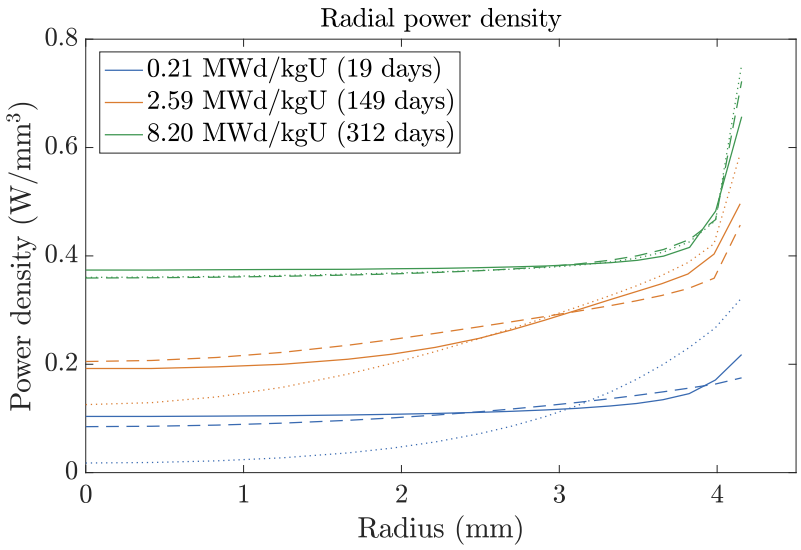

Figure 10: Radial power density distribution in the middle part (Slice 6) of the gadolinium-doped fuel rod at different burnups. Coupled calculation results are plotted with solid lines, standalone TRANSURANUS calculation results obtained with the default Gd model (option 1) with dotted lines and with a configuration-specific Gd model (option 102) with dashed lines. The burnup values are rod-average burnups corresponding to the irradiation days in brackets.

the configuration-specific Gd model are shown for the power density in Figure 12 and for the temperature in Figure 13. These figures reveal the differences along the full rod length. In the following, it is considered that the coupled calculation results represent the reference solution to which the stand-alone TRANSURANUS results are compared to.

Looking at Figure 12, it is evident that the largest differences between the approaches can be seen at low burnups. As was already visible in Figure 10, the radial power distributions are tilted relative to each other. At the lowest burnup of 0.21 MWd/kgU the stand-alone calculation first underestimates the power from the pin center until the mid-radius, then shifts to overestimate, until again underestimating the power at the very edge of the fuel. The behaviour is the same along the full axial length of the rod. The second burnup state at 2.59 MWd/kgU also shows the tilt between the radial profiles but now the inner part of the fuel is overestimated and the near-edge

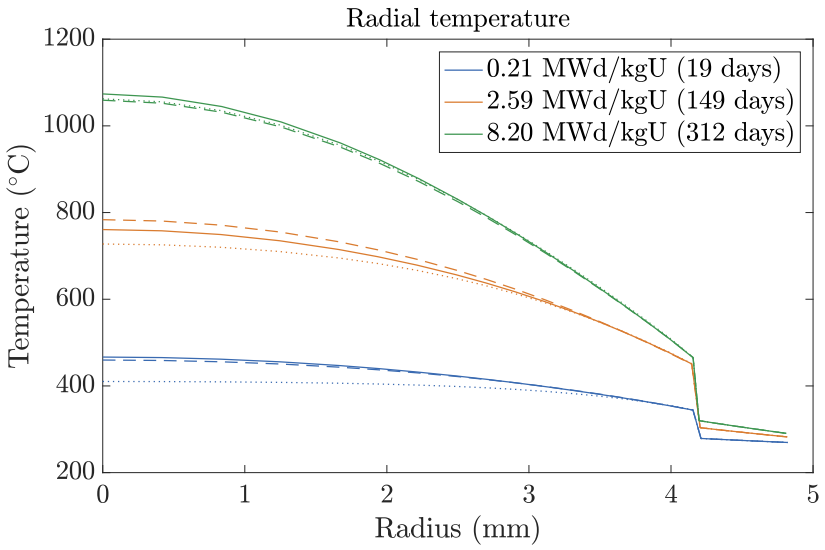

Figure 11: Radial temperature distribution in the middle part (Slice 6) of the gadolinium-doped fuel rod at different stages of the irradiation period. Coupled calculation results are plotted with solid and standalone TRANSURANUS calculation results obtained with the default Gd model (option 1) with dotted and with configuration-specific Gd model (option 102) with dashed lines. The burnup values are rod-average burnups corresponding to the irradiation days in brackets.

region underestimated with the shift being closer the the edge. The last two burnup states show that the underestimation visible for the major part of the fuel decreases as gadolinium burns, yet a clear overestimation still remains at the rim. There are also some differences in the axial direction. The largest under and over estimation are seen in the top and bottom axial sections at all burnup levels. The most likely explanation for the difference is that the radial power profiles calculated for these sections by Serpent in the coupled calculation are actually affected by the environment below and above the fuel (i.e. pin plenum, end plugs and moderator water). The internal radial power distribution solution in TRANSURANUS has no way of taking these into account. For comparison, although not presented as a separate figure, it should be noted that the differences in the power densities between the coupled calculation and the stand-alone TRANSURANUS calculation with the generic gadolinium model range from -60 % to 80 % at the burnup of 0.21 MWd/kgU and are still between -28 % and 18 % at the

burnup of 12.6 MWd/kgU.

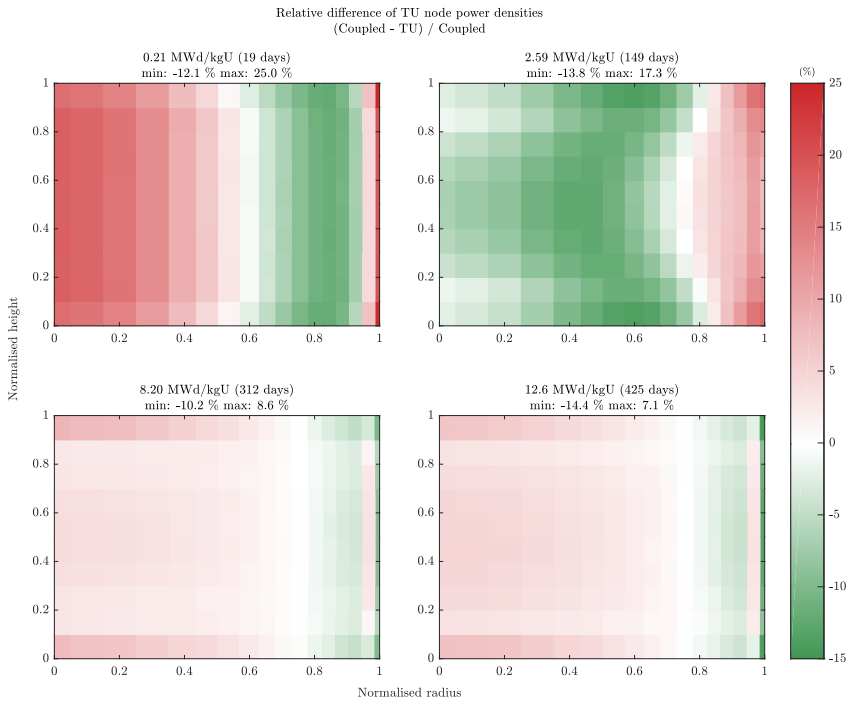

Figure 12: Relative difference of TRANSURANUS node power densities between a coupled Serpent-TRANSURANUS and a stand-alone TRANSURANUS calculation using a configuration-specific Gd-model (option 102) based on tabulated effective cross sections available in TRANSURANUS. The burnup values are rod-average burnups corresponding to the irradiation days in brackets.

The relative difference in the node temperatures between the coupled and stand-alone calculation results shown in Figure 13 visualise the effect the radial power distribution has on temperatures. The shift in the power density under/overestimation by the stand-alone TRANSURANUS calculation compared to the coupled calculation happening between the burnups of 0.21 MWd/kgU and 2.59 MWd/kgU is also seen as a shift in the temperature differences of the corresponding burnup states. Due to the close proximity of the thermal boundary condition, the temperature difference between the two approaches near and at the fuel edge is minimal. Thus, also the maximum differences between the coupled and stand-alone power distributions obtained at the rim

do not have a pronounced effect on the temperatures of this region. More importantly, whether the power level is under or overestimated in the bulk of the fuel appears to dictate whether temperatures are similarly under or overestimated. This is similar to the effect of a central hole in pellets, causing an outward displacement of the heat source in the pellet towards the heat sink (coolant), reducing the central temperature. To get also an idea of the actual scale of the temperature differences, the maximum local underestimation of 15 °C by the stand-alone calculation is obtained at 8.20 MWd/kgU and the maximum local underestimation of 23 °C at 2.59 MWd/kgU. For reference, the generic gadolinium model (option 1) predicts temperatures that differ from the coupled calculation results as much as 56 °C at low burnup and are still 23 °C at 12.6 MWd/kgU. This may not have large immediate implications from the safety point of view. Nevertheless, it is important for the accurate interpretation of experiments with fuel doped with neutron-absorbing isotopes in order to extract the correct temperature dependency of material properties such as the thermal conductivity.

5. Conclusions and Perspectives

A coupling between the fuel performance code TRANSURANUS and the Monte Carlo neutronics code Serpent was developed and implemented by means of an external driver program and making use of the features already existing in Serpent and TRANSURANUS facilitating data exchange between external codes. The coupled calculation system was tested in a realistic demonstration calculation based on a fuel performance benchmark with gadolinium-doped fuel.

As was seen in the results, the Monte Carlo neutron transport calculation is inherently capable of accounting for physical phenomena, such as the strong spatial self-shielding effects in burnable absorber containing rods, that simpler neutron diffusion based models stagger or need specific correction, for example, through configuration-specific effective cross section models such as available in TRANSURANUS. The differences in the radial form of the power are strongly reflected in the fuel temperatures. Comparing the results obtained using the generic and configuration-specific gadolinium model of TRANSURANUS to those obtained in the coupled calculation with the

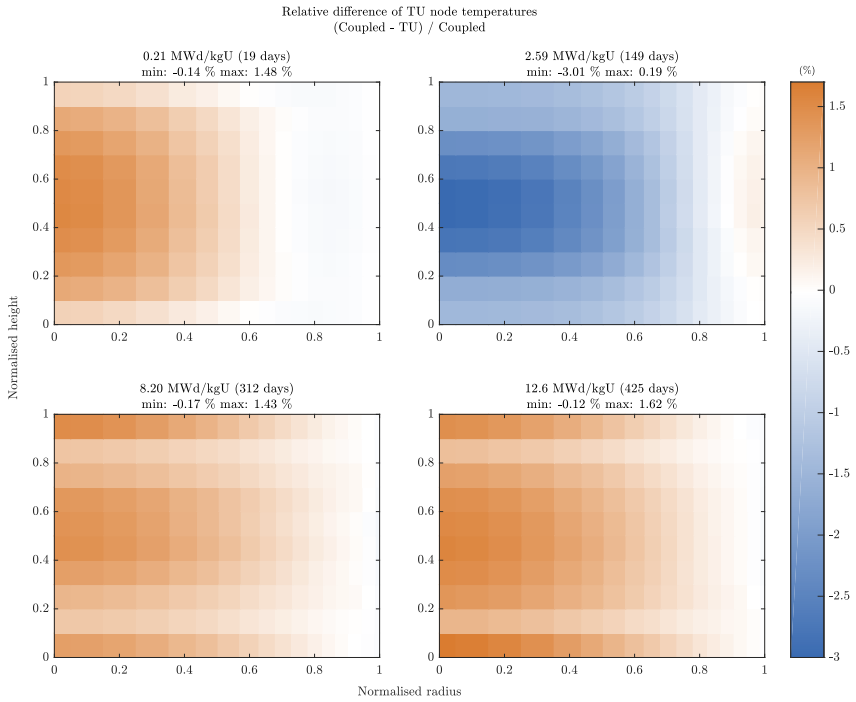

Figure 13: Relative difference of TRANSURANUS node temperatures between a coupled Serpent-TRANSURANUS and a stand-alone TRANSURANUS calculation using a configuration-specific Gd-model (option 102) based on tabulated effective cross sections available in TRANSURANUS. The burnup values are rod-average burnups corresponding to the irradiation days in brackets.

Monte Carlo neutronic solution, it seems obvious that when performing stand-alone fuel performance analyses one would prefer using the configuration-specific effective cross section models, even if only approximately related to the specific case, in place of the default generic Gd-model. The coupled scheme developed in this work can be used to develop such models (or to replace them altogether), as well as models for the new fuels such as so-called accident tolerant type of fuels.

Based on the results and convergence studies presented, the coupling methodology works as expected and can be utilised to produce reference level results that in the neutronic side account for rod internal temperature distribution and changes in the radius and in the fuel performance side replace simpler diffusion approximation-based

radial power distribution solutions with those obtained from a Monte Carlo neutron transport calculation. A Serpent calculation model can, in principle, be a fully three-dimensional representation of an entire reactor refined to an arbitrary level of detail. Serpent can also utilise the full energy dependence of the cross section data available. From the viewpoint of a fuel performance code coupled with Serpent, these features mean that a very realistic estimate for the power distribution in the rod of interest can be obtained. In practice, however, due to the high computational effort required by the Monte Carlo neutron transport calculations especially when resolving the internal power distribution of fuel pins, the calculation model in most cases will likely consist, at most, of a single fuel assembly with the rod(s) of interest, possibly including details of the immediate neighbourhood for improved boundary conditions. Provided sufficient computing resources, larger scale coupled calculations could be attempted as the Monte Carlo neutronics in general scales well. However, the memory requirements also increase due to the increased number of depletion regions. This would likely require further development in Serpent, for example, in the form of domain decomposition based parallel calculation capabilities to reduce the memory requirements for a single computing node. In such a case it would make sense also to parallelise the fuel performance calculation of the separate fuel pins.

As this type of coupled calculations are very time consuming, instead of routine fuel performance analyses at nuclear plants, the use may be limited to more research-oriented applications and special purposes. For example, the coupled scheme could be applied for the high-fidelity simulation of separate-effect experiments with special fuel discs in a research reactor, where the special configuration or material compositions demand a detailed neutronic calculation instead of a simplified diffusion approximation. One should keep in mind, however, that beyond the radial power profile, such specific configurations may also require to consider higher dimensional heat transfer and stress calculations. In order to reduce the total calculation time, one could consider the application of a more refined radial mesh towards the pellet rim by means of a dichotomic instead of an equi-volume discretisation. Another important reduction of the calculation time could be achieved when combining the less accurate Monte Carlo results directly with a radial piecewise linear fitting tool in the FRAToolbox (Lassmann et al.,

2015) for example. The loss of information in the less accurate Monte Carlo results could be compensated by the powerful piecewise fitting tool with moving windows. Yet another way could be to replace the bin-based tallies in Serpent altogether with a polynomial function based approach by utilising functional expansion tallies. Preliminary work towards this direction has already been started as described by Suikkanen and Rintala (2019).

As for further improvement of the coupled calculation system, a thermal-hydraulic solver could be included to the coupling to provide a calculated thermal boundary condition for the fuel rod calculation as well as coolant temperature and density for the neutronics part. Another potential development would be to include isotope concentration data calculated by Serpent to the fuel performance code, essentially replacing the whole nuclide analysis module of TRANSURANUS by that of Serpent.

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