



Serpent-ENIGMA - Combining Monte Carlo Reactor Physics with Fuel Performance

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<p>Summary</p> <p>This report documents the coupling of Monte Carlo Reactor physics code Serpent to the fuel performance code ENIGMA. The new coupling code SEN uses ENIGMA to model the dynamical behaviour of the fuel, i.e. changes in the fuel dimensions and temperature distribution. SEN forwards this information to Serpent that is used to calculate the power distribution and burnup of the fuel. The radial power distribution data is returned to ENIGMA to be utilized by its power depression routines.</p> <p>SEN provides for detailed temperature and geometry modelling in a burnup calculation. Hence, it can be utilized to realistically estimate the errors originating from the usual approximation of stationary thermo-mechanical properties. The new code can also be used in the validation of different models and input parameters of ENIGMA. Additionally, the automatic power distribution calculation capability is handy in the fuel performance modelling of gadolinia-doped fuel rods.</p> <p>SEN was tested with a realistic PWR fuel rod case from the FUMEX research program. The results showed that the effect of thermo-mechanical properties on the results of a burnup calculation is small, but not fully insignificant.</p>		
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1 Introduction

Whenever a fuel rod is irradiated in a nuclear reactor, the fuel and cladding materials are exposed to high temperatures, temperature gradients, high pressures and neutron flux. The harsh conditions inflict significant changes in the fuel behaviour and, therefore, the understanding and prediction of these changes is essential for safe and economical operation of nuclear reactors.

Time development of the fuel and the reactor as a whole is being researched using different kinds of calculation codes. Reactor physics codes are used to predict the multiplication factor and power distribution of the reactor, along with many other important parameters. Some reactor physics codes also include a burnup calculation capability, which makes it possible to calculate the neutron flux – induced changes in the nuclide inventory and, consequently, provides for rather accurate modelling of the time evolution of the reactor.

Another important branch of codes consists of the fuel performance codes that are meant especially for modelling the thermo-mechanical behaviour of nuclear fuel. They predict, for instance, the changes in fuel rod dimensions, thermal conductivity, temperature and fission gas release along with fuel long-term irradiation (steady-state codes) or in transient conditions (transient codes). The main purpose of these codes is to ensure that the fuel rods do not fail during normal operation or transients, mainly by checking that certain safety limits are met in all conditions.

Traditionally, fuel performance calculations and reactor physics have been strictly separated from each other. When making fuel performance calculations, the reactor physical parameters such as power distribution, fission gas production and fast flux are either calculated externally and given to fuel performance codes as input or calculated directly by fuel performance codes using approximate models. At the same time reactor physics calculations are usually performed as if the thermo-mechanical properties of the fuel would remain constant over the whole irradiation period. The amount of error caused by this approximation is a rather unknown subject, which this study tries to explore.

The current study yields a new coupling code for performing combined fuel performance and reactor physical calculations. The code is christened “SEN” after the reactor physics code Serpent and the steady-state fuel performance code ENIGMA it couples. SEN makes it possible to evaluate the magnitude of error caused by thermo-mechanical changes in the fuel rods during irradiation. SEN also provides for an easy way of calculating the accurate power distribution and the fast flux that are important and sometimes hard-to-find input parameters for ENIGMA.

This document summarizes the development of SEN. Section 2 contains a small introduction to the codes Serpent and ENIGMA on which SEN is based, Section 3 describes the methodology of SEN. Results obtained with SEN are presented in Section 4, Section 5 is left for conclusions and the whole document is summarized in Section 6.

2 Codes behind SEN

The basic idea of SEN is to extend the capabilities of ENIGMA by introducing some parameters from the reactor physics code Serpent. Input of SEN is practically the same as that of ENIGMA: only fuel rod pitch and a couple of special parameters for Serpent must be given outside of a standard ENIGMA input. Consequently, SEN should be easily adoptable by professionals already familiar with ENIGMA.

2.1 Fuel performance code ENIGMA

ENIGMA is a steady-state fuel performance code developed by Nuclear Electric and BNFL in the United Kingdom [1]. The code has been widely used at VTT for many years. The version currently in use at VTT is based on ENIGMA version v.5.9b, but the code has been further modified. Most of these modifications are model extensions and additions concerning, for example, cladding material properties, fission gas release and gadolinia-doped fuel rods [2].

The modification most relevant to the current work is a new radial power profile capability that was implemented in 2009 [4] by Libor Klecka. The new routine reads the radial power distribution from a separate input file and, thus, provides for external power profile calculation. The capability was originally meant for Gd-doped fuel rods in such a way that power distributions at different burnups are pre-calculated with a reactor physics code, but the same routine can also be utilized to update the power profile between irradiation steps of an ENIGMA calculation.

ENIGMA was slightly modified during the development of SEN. Most of the modifications were related to the (new) compilation of ENIGMA in Linux environment and re-enabling of the restart feature that had been forgotten in the implementation of a few of the newest ENIGMA modifications by VTT.

The previous version of ENIGMA also included a bug – or at least incoherence - concerning burnup normalization in rods containing gadolinia. The gadolinia content was not taken into account in the calculation of uranium mass (part of the uranium is replaced by gadolinia), which led to too high uranium mass and, furthermore, too small burnup when compared to linear power and irradiation time. The effect of gadolinia content on burnup normalization of ENIGMA was fixed, but it was recognized that gadolinia content may have significant effects also in some other parts of the code. These effects should be investigated thoroughly before the results from Gd-rods can be kept as confident as those from non-Gd rods.

2.2 Monte Carlo reactor physics code Serpent

Serpent is a novel Monte Carlo reactor physics code developed by Jaakko Leppänen at VTT. The code is optimized for group constant creation in two-dimensional lattices, but it is also capable of three dimensional calculations. The code includes a burnup calculation capability, which makes it possible to

investigate time evolution of the nuclear fuel. At the moment Serpent has users in more than 40 organizations around the world [5,6].

3 The new coupling code SEN

SEN reads parameters from an ordinary ENIGMA input and splits the N-step irradiation history defined in ENIGMA input to N separate irradiation steps using the restart property of ENIGMA. SEN utilises Serpent to update the radial power distribution between the irradiation steps. Since SEN creates the Serpent inputs according to the real time fuel rod state information calculated by ENIGMA, the thermo-mechanical properties become correctly taken into account in the Serpent simulations. SEN executes the programs Serpent and ENIGMA automatically as the up-to-date input files have been created.

By default the Serpent inputs describe a pin cell situated in an infinite lattice. It is, however, easy to extend the simulation to more complicated geometries as it is described in the next subsection.

3.1 Input

The input of SEN has three parts. SEN is run on command line by typing

```
sen < ENIGMA input file > < reduced Serpent input >
```

where the <ENIGMA input file> is just an ordinary ENIGMA input file with control data, keyword input and history input. It should be noted that the number of rings and number of axial zones used in the Serpent simulations are the same as stated in the ENIGMA input. Hence, division to numerous annular zones increases the memory consumption of Serpent significantly. Also the running time of SEN is multiplied by the number of axial zones, because each axial zone is modelled separately with Serpent due to power normalization issues.

The Serpent input file should contain all instructions for Serpent that are not directly related to the geometry or materials of the fuel pin being modelled. The minimum requirements for the contents of this file are

- Neutron population (for example, `set pop 1000 200 20`)
- Boundary condition (`set bc 3`)
- Cross section library (`set acelib "sss_jeff311u.xsdata"`)
- Fission yield and decay libraries (`set declib...`, `set nfylib ...`)
- Some options for burnup calculation:
 - o `set pcc 1` – enable predictor-corrector calculation
 - o `set printm 1` – print material compositions after each step

Advanced users of SEN may utilize the reduced Serpent input file for many other things such as

- Modelling of geometries other than pin cell

- The standard Universe of the fuel pin can be modified in include.h header file
- Remember to add a “set bunorm 2” card if the geometry contains fissile materials other than the pin. This causes the power to be normalized to the pin only if it is the only burnable material in system.
- Include.h contains also possibilities for multiplication of the examined rod and power multiplication in case there are multiple burnable materials within the problem geometry.
- Reduction of energy grid size
- Creation of group constants
- Geometry and / or mesh plots
- Cut-offs.
- Detector options
- Etc...

The third part of the input is given to SEN in stdin: the program asks for the fuel rod pitch in centimetres. An easy way to give this parameter is to start the SEN program as

```
echo "1.23" | sen ENIGMA.inp serpentinp
```

3.2 File naming conventions and output

SEN uses the body of the ENIGMA input file as a basis name for all the input and output files. For example, if an ENIGMA input file is named “fumex.inp”, the <body> of the file is simply “fumex” without the quotation marks.

As was previously mentioned, SEN splits the ENIGMA run defined in <body>.inp to smaller ENIGMA simulations that are run one by one. Input files of these mini simulations are named <body>.sSS.inp, where SS is the irradiation step number expressed by at least two integers. ENIGMA restart information for each step is stored in files <body>.rstS, where S is again the irradiation step number. Outputs of the ENIGMA calculations can be found in files <body>.op* and <body>.z*, but only for the last step since the old op-files are overwritten during the SEN run. It is easy to repeat the calculation for an arbitrary step since the restart information files and ENIGMA inputs are available for each step. More information on the output files of ENIGMA can be found in Ref. [7].

Serpent input files are named <body>.sSSzZ, where SS is the irradiation step number expressed with at least two digits and Z is the number of axial zone. Multiple output files are produced for each of the Serpent runs. More information on the output files of Serpent can be found in Ref. [8].

The main output file of SEN is named <body>out.m. The file is in Matlab format and the contents of this file are summarized in Table 1.

Table 1. Contents of the Matlab-formatted inputfile <body>out.m.

INPUTFILE_BODY	Body of the input file.
SERPENT_TEMPLATE	Name of the reduced Serpent input file.
DENSITY_AT_BOL	Fuel density at beginning of life (proportion of

	theoretical).
ENRICHMENT	Uranium enrichment (weight proportion of U-235).
PITCH	Fuel rod pitch (cm)
GDCONTENT	Proportion of gadolinia of total fuel weight.
ZONE_LENGTHS	Axial zone lengths. (cm)
STEP_LENGTHS	Irradiation step lengths.(hour)
COOLTEMPS(:,:)	Coolant temperatures for each axial zone and step.
LINPOWERS	Linear power ratings for eah axial zone and step. (W/cm)
CUMUL_BURNUPS	Cumulative burnups for each axial zone in MWd/tU at end of irradiation steps. Calculated straight from linear powers and fuel mass. End of step values (EOS). (MWd/tU)
OUTRADIUS	Ring outer radii for each step (:,x,x), axial zone (x,:,x) and ring (x,x,:). Half step values (HS). (cm)
INRADIUS	Ring inner radii for each step, axial zone and ring. HS. (cm)
RELPOW	Serpent-calculated relative powers for each step (:,x,x), axial zone(x,:,x) and ring(x,x,:).
ENIGMA_RELPOW	Relative powers used by ENIGMA.
T	ENIGMA-calculated average temperatures for each step, axial zone and ring. HS. (K)
TMC	Monte Carlo temperatures used in Serpent calculation for each step, axial zone and ring. (Kelvin)
BURNUP	Regional burnups for each step (:,x,x), axial zone (x,:,x) and ring (x,x,:) as calculated by Serpent. EOS. (MWd/tU)
BURNUP_ENIGMA	Regional burnups for each step, axial zone and ring as calculated by ENIGMA. EOS. (MWd/tU)
DENSITY	Regional densities for each step, axial zone and ring. Calculated from changes in regional volumes assuming mass conservation. HS. (g/cm ³)
KEFF	Keff and proportional error. Beginning of step values (BOS).
ENIGMA_AVGBURNUP	Average burnups for each burn step as calculated by ENIGMA. EOS. (MWd/tU)
CENTERLINE_TEMP	Fuel centerline temperatures for each step and axial zone. HS. (Kelvin)
FFLUX	Fast flux for each step and axial zone as calculated by Serpent. BOS. (n/cm ² s)
ENIGMA_FFLUX	Fast flux for each step and axial zone as calculated by ENIGMA on the basis of input. HS. (n/cm ² s)
RELEASE	Non-cumulative fission gas releases for each step, axial zone and ring. HS.

3.3 Detailed description of SEN

A SEN run begins by reading the initial parameters of the fuel rod and irradiation history information from the ENIGMA input. On the basis of this data, SEN

creates the geometry, detector and initial material inputs for the first Serpent calculation. The reduced Serpent input file is copied in between geometry and material definitions without any modifications.

For this initial step the temperature distribution is unknown. Therefore, the whole fuel rod is assumed to be in the coolant temperature.

After the first Serpent run the heat production data is read from Serpent output. SEN utilizes this data in the creation of a radial power input file for ENIGMA. Format of the file is described in Ref. [4]. After this, ENIGMA is run for half a step. New fuel dimensions and the temperature distribution are read from its output. The half step values of the temperature distribution and fuel dimensions are considered here the most representative values for the whole step.

Since the first Serpent run was made with an unrealistic zero-power temperature profile and cold dimensions, the first Serpent run is repeated with updated data from the ENIGMA output to obtain more reliable results. After the power profile input file is updated according to the new calculation, ENIGMA is run for a whole irradiation step and its output is stored.

The SEN run continues with the consequent steps. For each step ENIGMA is first run for a half step to get the temperature distribution and dimensions corresponding to the momentary linear power, then Serpent is run with these dimensions and, finally, the irradiation step ends with an ENIGMA run for a full irradiation step. The program flow is sketched in Figure 1.

3.3.1 Reduction of temperatures

ENIGMA calculates an average temperature for each annulus in the geometry. It would be possible to forward this temperature information to Serpent in the raw, but handling multiple temperatures in Serpent consumes huge amounts of memory. Therefore, it is in many cases convenient to reduce the number of temperatures for the Monte Carlo calculation.

SEN has two possible methods for reducing the number of different temperatures. If the `MAX_TEMPERATURES` -parameter in `include.h` is smaller than the number of annuli in the fuel but greater than one, the number of different temperatures is reduced by repeatedly combining temperatures of two adjacent annuli. The temperature in the new temperature zone is chosen as the volume-averaged value of the combined zones. Two annuli with the smallest temperature difference are combined repeatedly until the number of different temperatures equals `MAX_TEMPERATURES`.

If `MAX_TEMPERATURES` equals one, SEN utilizes a widely-used effective temperature formula known as the Rowlands formula [9]. The formula calculates a chord-averaged average temperature for the fuel rod assuming that the temperature distribution is r^2 -shaped.

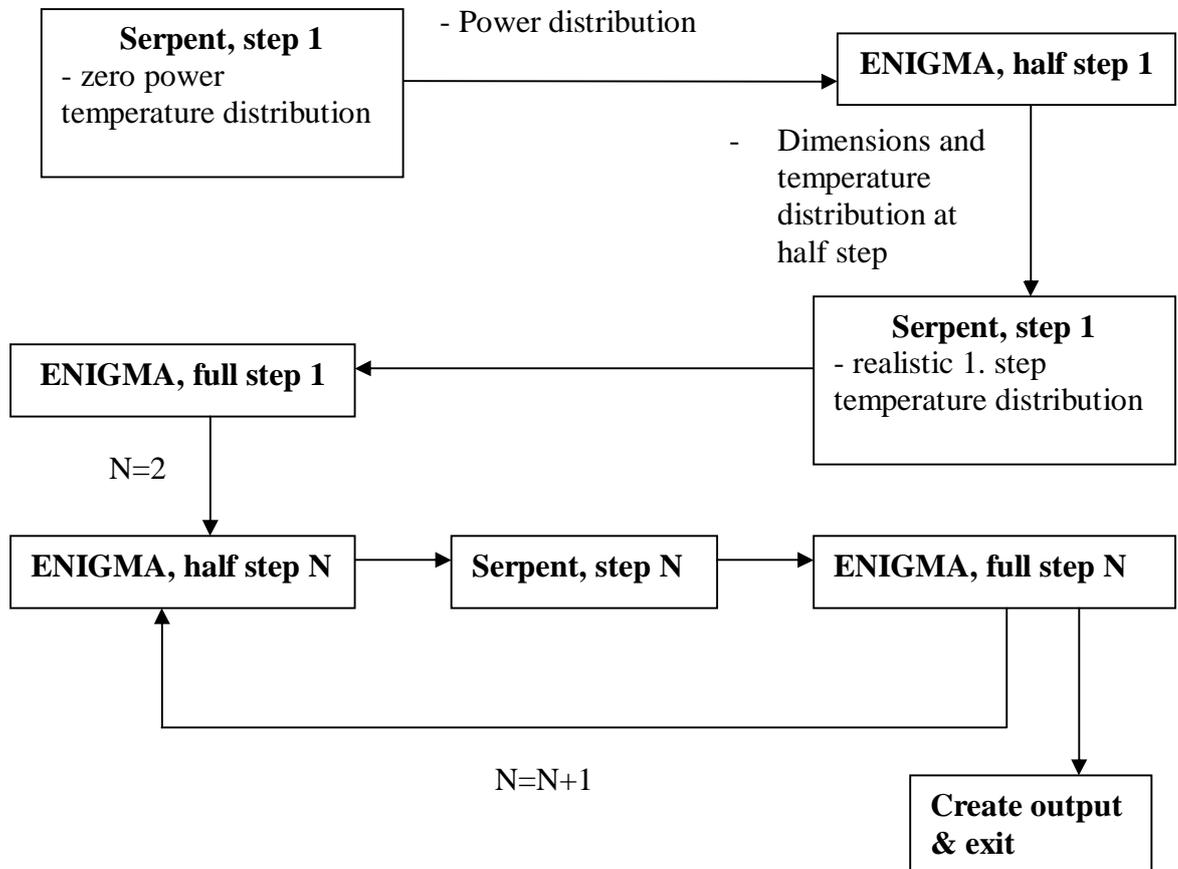


Figure 1: The program flow of SEN. The code creates inputs for each of the simulations and executes the programs ENIGMA and Serpent automatically.

4 Results

To gain realistic information on the significance of coupled fuel performance and neutronics modelling, a benchmark PWR rod from the IAEA Coordinated Research Programme FUMEX-III (Fuel Modelling at Extended burnups) was simulated with Serpent, ENIGMA and SEN, separately. The rod is a common PWR rod with fuel enriched to 3.48 w-% U-235. The maximum burnup at the centre of the rod reaches about 52 MWd/kgU at the end of irradiation.

The template of the ENIGMA input has been previously created by Ville Tulkki for simulations related to the FUMEX benchmark project [3]. In this input the number of radial regions was reduced to 15, or to 5 in case of the results presented in Section 4.2, and the number of axial zones was reduced to 2 to speed up the calculations and simplify the analysing of the results. All of the Serpent simulations were performed in the pin cell geometry that is illustrated in Figure 2.

To get as diverse results as possible, first of the two axial zones was chosen as the segment at the lowermost ending of the rod and second of the zones was chosen

from the middle, where the linear power ratings are maximal. Because of the artificial reduction of fuel zones in axial direction, the ENIGMA modelling of axially coupled effects, i.e. internal pressure, fission gas release and elongation, is no longer realistic. Regardless, the results should provide rather reliable information about the magnitude of errors caused by assuming the fuel properties to be stationary.

All of the calculations were made with `MAX_TEMPERATURES = 5`. The input files are Appendices A-B.

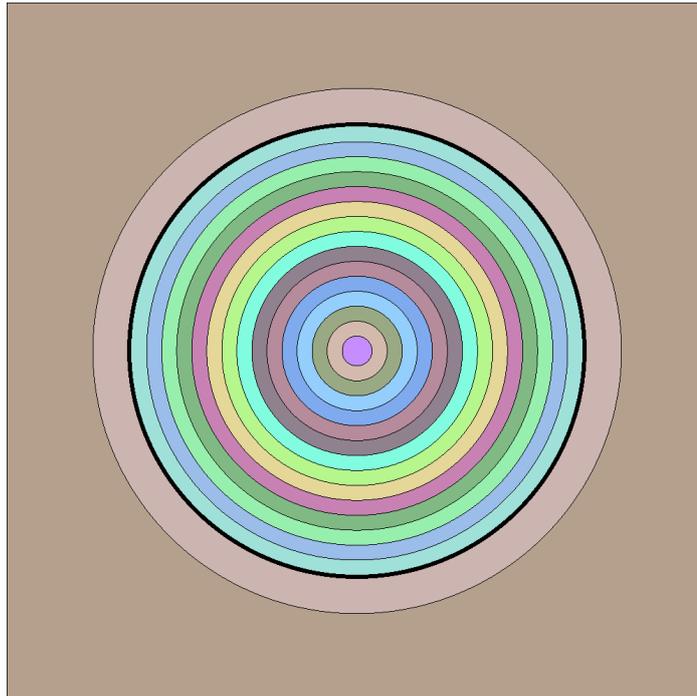


Figure 2: The pin cell of the FUMEX fuel rod. In this figure the fuel part is divided into 15 annular zones with equal radii. The gas gap and cladding can also be recognized in the figure.

4.1 Comparison of SEN to Serpent

Effect of the dynamical fuel behaviour on neutronics can be estimated by performing the burnup calculation separately with SEN and Serpent. In the Serpent simulation, the initial fuel geometry and the temperature distribution corresponding to the linear power of the first irradiation step are utilized throughout the irradiation history. It should be noted that these first step values are most probably not the most representative choices for the whole history, but they are utilized here mainly for demonstration purposes.

The results are compared via homogenized one-group fission and capture cross sections of the fuel pin cell. Results for the lowermost rod segment are presented in Figure 3 and for the middle segment in Figure 4.

Additionally, the cases were simulated with two special versions of SEN that kept either the geometry or the temperature constant over the irradiation period. Results of these special cases are presented in Appendix C.

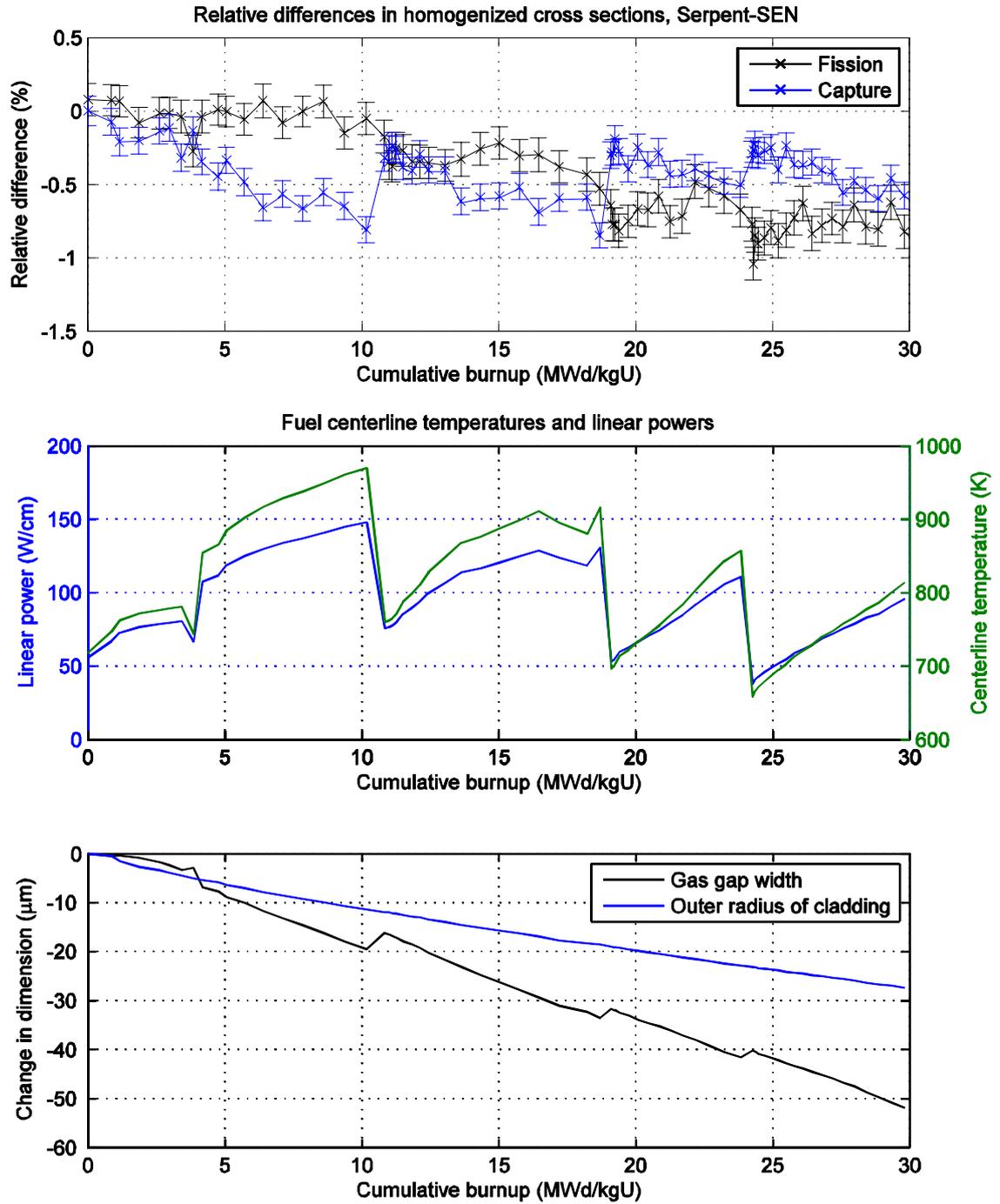


Figure 3: Selected results for the lowermost fuel rod segment, which is irradiated at quite a low linear power.

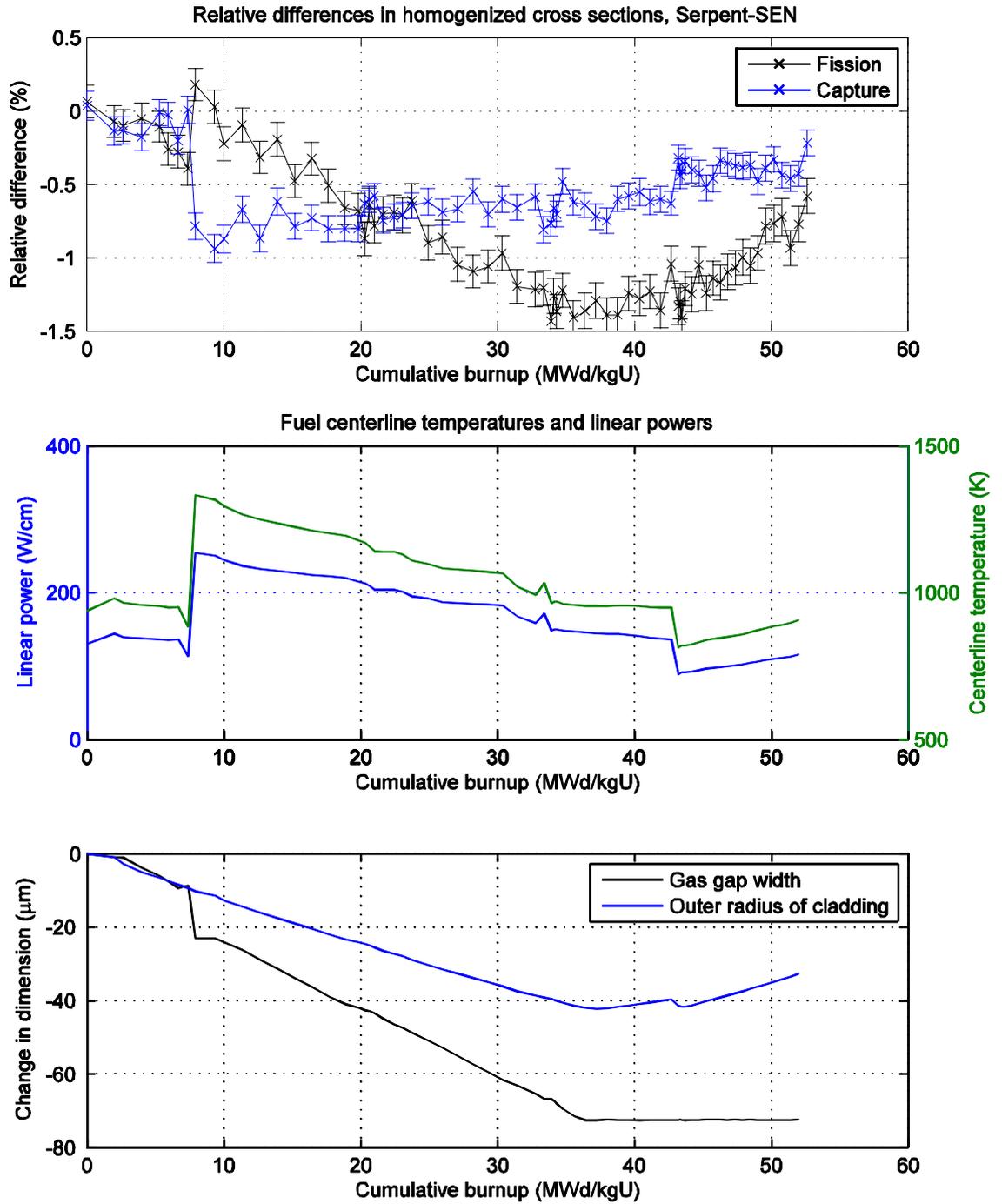


Figure 4: Selected results for the middle rod segment for which the linear powers are the highest.

4.2 Power depression models of ENIGMA

Even though the main emphasis of this work was on finding out the effect of the dynamic behaviour of fuel on neutronics, SEN also provides for an easy way of validating the radial power depression models of ENIGMA. The FUMEX case was first modelled with ENIGMA using the built-in RAD99 power depression model. The results are compared to a SEN simulation of the same case. SEN utilizes the external power distribution model and resolves the power depression using Serpent.

Perhaps the easiest way of examining the overall performance of the power depression models is through burnup distributions at the end of the simulation. Burnup distribution is, thus, obtained from the power distribution via integration over time. The final burnup distributions for the two fuel segments are compared in Table 1.

Table 1: Comparison of the final burnup distributions for the two fuel segments.

Lowermost segment				Middle segment			
	ENIGMA	SEN	difference		ENIGMA	SEN	difference
	MWd/tU	MWd/tU	%		MWd/tU	MWd/tU	%
ring 1 (out)	32501	32799	0,91	ring 1 (out)	59158	58833	0,55
ring 2	28690	28516	0,61	ring 2	49243	49188	0,11
ring 3	27842	27718	0,45	ring 3	47262	47663	0,84
ring 4	27515	27334	0,66	ring 4	46593	46976	0,82
ring 5 (in)	27373	27069	1,12	ring 5 (in)	46317	46479	0,35
avg.	29575	29575	0,00	avg.	51861	51861	0,00

5 Conclusions

5.1 Comparison to Serpent

The results in Figures 3 and 4 represent two fuel segments with rather different linear power histories. In case of both of the segments a slight dependence of homogenized cross sections on the thermo-mechanical properties can be recognized. By examining the corresponding results of the distinct runs, presented in Appendix C, it can be noticed that both the changing geometry and the varying temperature have their own contributions to the differences.

As can be seen in the middle plots, the correlation between linear power and temperature of the fuel is very strong. Since the linear powers in the very beginning of the irradiation history are small compared to the later history, also the fuel temperatures in the Serpent case remain smaller almost throughout the whole history.

The higher fuel temperature increases the resonance absorption in the fuel material, mainly U-238, because of Doppler-broadening of the resonance peaks.

As a consequence, the capture cross section increases suddenly in the SEN case along with linear power as can be seen in the cross section curves.

A long-term consequence of the heightened resonance absorption is that new fissile material, mainly Pu-239 and Pu-241, is created in the fuel more efficiently than in the cooler case. Extra fissile material tends to increase the fission cross section of the SEN case above that of the pure Serpent calculation. For example, at 40 MWd/kgU the Pu-239 content of the middle segment fuel rod was about 2 % higher in the SEN calculation than in the Serpent case.

The effect of the varying geometry can be recognized in Figure 6 of Appendix C. In this high linear power case cladding creep increases the volume of the water channel between the fuel rods until the gas gap closes at around 36 MWd/kgU after which the cladding starts to slowly expand. The increase in water channel volume enhances the moderation slightly and, thus, might be reason for the increase in both fission and capture cross sections compared to the Serpent case.

On the other hand, also the swelling of the fuel material itself may have some effect on the cross section. From the current results it is impossible to conclude at full confidence, which is the primary cause for the differences seen in cross sections.

In general, the cross section errors in Figures 3 and 4 remain below 2 percents, which is considered a small but not fully insignificant magnitude for errors. The errors in the burnup calculation of Serpent could be decreased by utilizing a more representative temperature distribution for the run, for instance a distribution from the middle of the irradiation history.

5.2 Power depression models of ENIGMA

The results in Table 1 clearly indicate that at least in this PWR case the RAD99 power depression model of ENIGMA is very accurate. All of the differences remain below 1 percent except for the inner ring of the lowermost segment for which the error in burnup reaches 1.12 percents.

Most probably the RAD99 model would fail if the PWR rod was doped with gadolinia, which significantly affects the power profile especially at the beginning of the irradiation. To provide for proper modelling of Gd-doped rods, an external power depression capability (FILE option) has been previously implemented in ENIGMA [4].

5.3 Future prospects

SEN might be of great help for ENIGMA users. SEN can easily provide information on the fast flux and power distributions in arbitrary fuel rods. The developers of ENIGMA might also find the ability to calculate the exact fission gas composition useful.

To help the ENIGMA users, it might be a good idea to hide the Serpent input part by hard-coding the necessary Serpent input information within SEN. This way the

usage of SEN would become trivial for the professionals already familiar with ENIGMA. The SEN output should also be clarified in case the code would be used widely in the future.

SEN could also be optimized in many ways. It is, for example, inefficient to use the same time step division for the neutronics and fuel performance calculations. In many cases it should be possible to use a sparser division for the Serpent calculations without significantly affecting the accuracy. Another potential way of reducing the calculation intensity of SEN would be to decrease the number of axial zones for which the neutronics calculation is made. The reduction could be executed by averaging the material compositions, linear powers and coolant temperatures over a few adjacent axial zones and using the averages in the neutronics modelling.

6 Summary

Monte Carlo Reactor physics code Serpent was successfully coupled with the fuel performance code ENIGMA by writing a coupling code named SEN. The new code uses ENIGMA to model the dynamical behaviour of the fuel, i.e. changes in the fuel dimensions and temperature distribution. SEN forwards this information to Serpent that is used as a burnup and power distribution calculator. The radial power distribution data is returned to ENIGMA to be utilized by its power depression routines.

SEN provides for detailed temperature and geometry modelling in a burnup calculation. Hence, it can be utilized to estimate the errors originating from the usual approximation of stationary thermo-mechanical properties. The new code can also be used in the validation of different models and input parameters of ENIGMA. Additionally, the automatic power distribution calculation capability is very handy in the fuel performance modelling of gadolinia-doped fuel rods.

SEN was tested with a realistic PWR fuel rod case from the FUMEX research program. The results showed that the effect of thermo-mechanical properties on the results of a burnup calculation is small, but not fully insignificant.

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Appendix A: ENIGMA input for the FUMEX PWR rod

16x16 US PWR TSQ004
ZIRC
2 15 0
AXIAL ZONES FLAG = SAME
HISTORY FLAG = MULTIZONE1
HISTORY TYPE FLAG = ENIGMA
RATING UNITS FLAG = KW/M
POWER DEPRESSION FLAG = RAD99
CLAD CREEP FLAG = SL82
CLAD YIELD STRESS
330.
COOLANT PRESSURE
15.5 0.0
ENRICHMENT
.0348
GADOLINIA CONTENT
0.00
FUEL GRAIN SIZE
1.E-05
FUEL POROSITY
0.05
0.
PELLET GEOMETRY
0.003 0.005
PELLET LENGTH
0.0099
PELLET RADIUS
0. 0.0041275
CLAD RADIUS
0.0042164 0.0048514
PLENUM
2.62 25.4E-06 400.
POWER
0.974 3.2E+16
* Fast flux is highly speculative
CLAD CREEP
1.5E-3 1.5 .33 7070
2.0E-23 .0082 7070
ZONE LENGTH
0.1524 0.1524
END OF KEYWORD DATA
1747.200000
290.000000 306.000000
5.600000 13.000000
0
2272.800000
290.000000 306.000000

```
6.700000 14.400000
0
3388.800000
290.000000 306.000000
7.300000 13.900000
0
4504.800000
290.000000 306.000000
7.700000 13.700000
0

...
-- 62 steps of irradiation history removed from here --
...

39386.400000
290.000000 306.000000
9.600000 11.600000
0
```

Appendix B: Reduced Serpent input file for the FUMEX PWR

```
set title "2-dimensional PWR rod in a pin cell"

set acelib "/home/tpvtuomas/xsdata/sss_jeff311u.xsdata"

% --- Periodic boundary condition:

set bc 3

% --- Group constant generation:

% universe = 0
% symmetry = 0 (no symmetry)
% 2-group structure (group boundary at 0.625 eV)

set gcu 0
set sym 0
set nfg 2 0.625E-6

% --- Neutron population and criticality cycles:

set pop 5000 500 20

% --- Geometry and mesh plots:

plot 3 1000 1000
mesh 3 1000 1000

% --- Data libraries for burnup calculation ---
```

```
set declib "/home/tpvtuomas/xsdata/sss_jeff311.dec"
set nfylib "/home/tpvtuomas/xsdata/sss_jeff311.nfy"

% --- Reduce energy grid size:

set egrid 5E-5 1E-9 15.0

% --- Cut-offs:

set fpcut 1E-6
set stabcut 1E-12

% --- Options for burnup calculation:

set bumode 2 % CRAM method
set pcc 1 % Predictor-corrector calculation on
set xscal 2 % Cross sections using main grid

set printm 1 % Print compositions after each step

set bunorm 2 % Normalize power to burnable materials only

% --- Burnup steps

set inventory

922350
922380
942390
```

Appendix C: Additional results

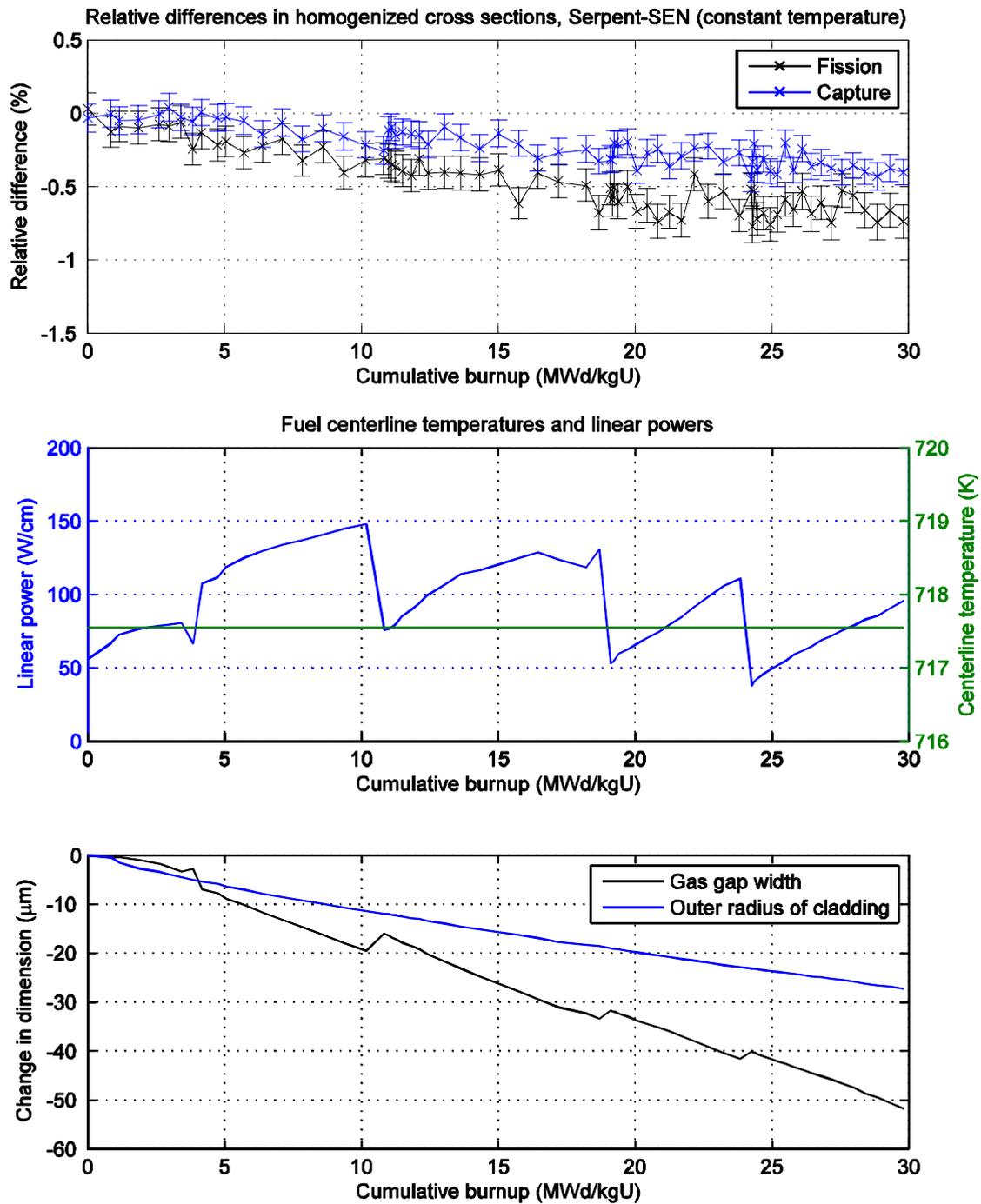


Figure 5: Results of a special SEN simulation in which the temperature was kept constant and only geometry was varied. Low linear power case.

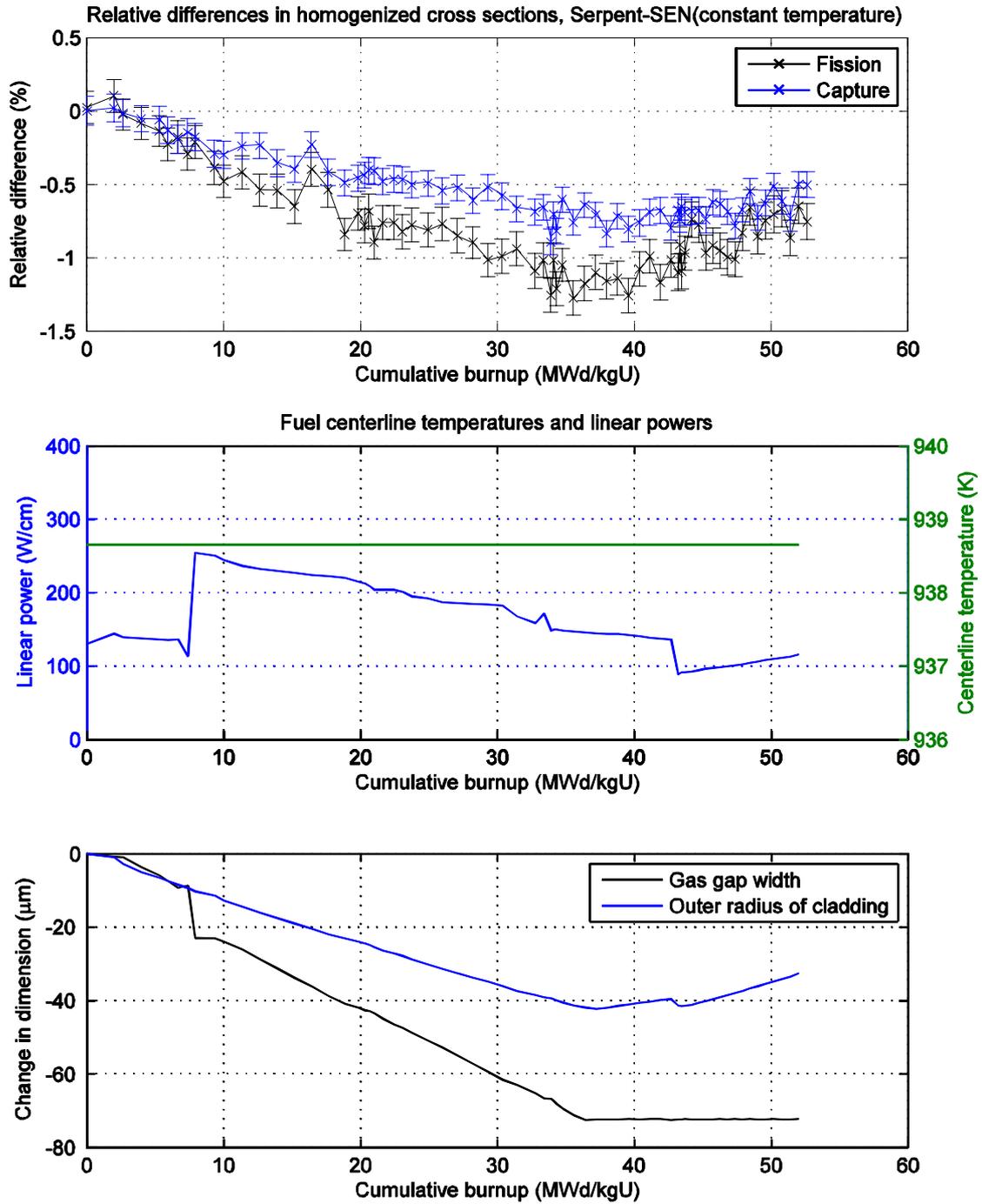


Figure 6: Results of a special SEN simulation in which the temperature was kept constant and only geometry was varied. High linear power case.

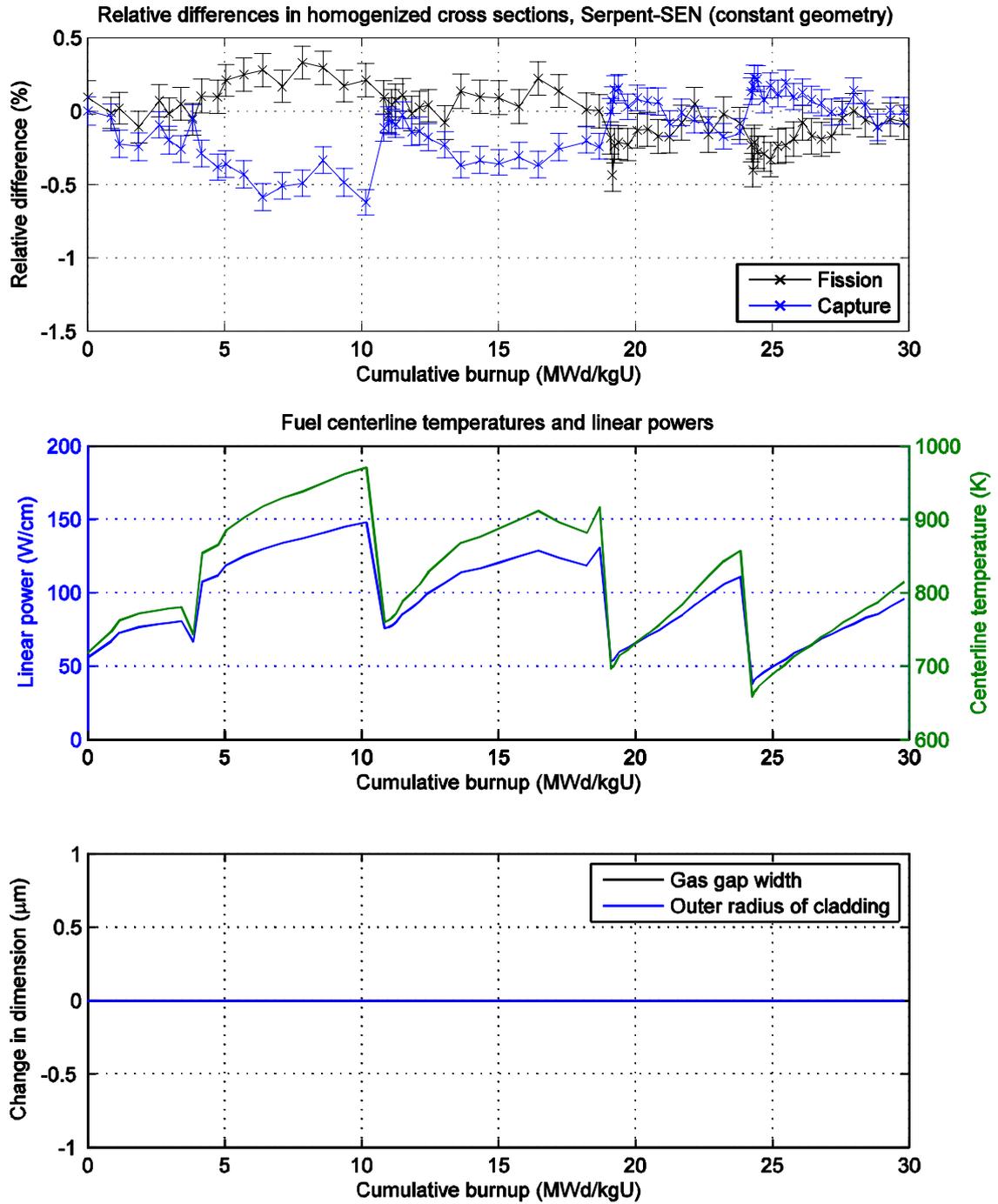


Figure 7: Results of a special SEN simulation in which the geometry was kept constant and only temperature was varied. Low linear power case.

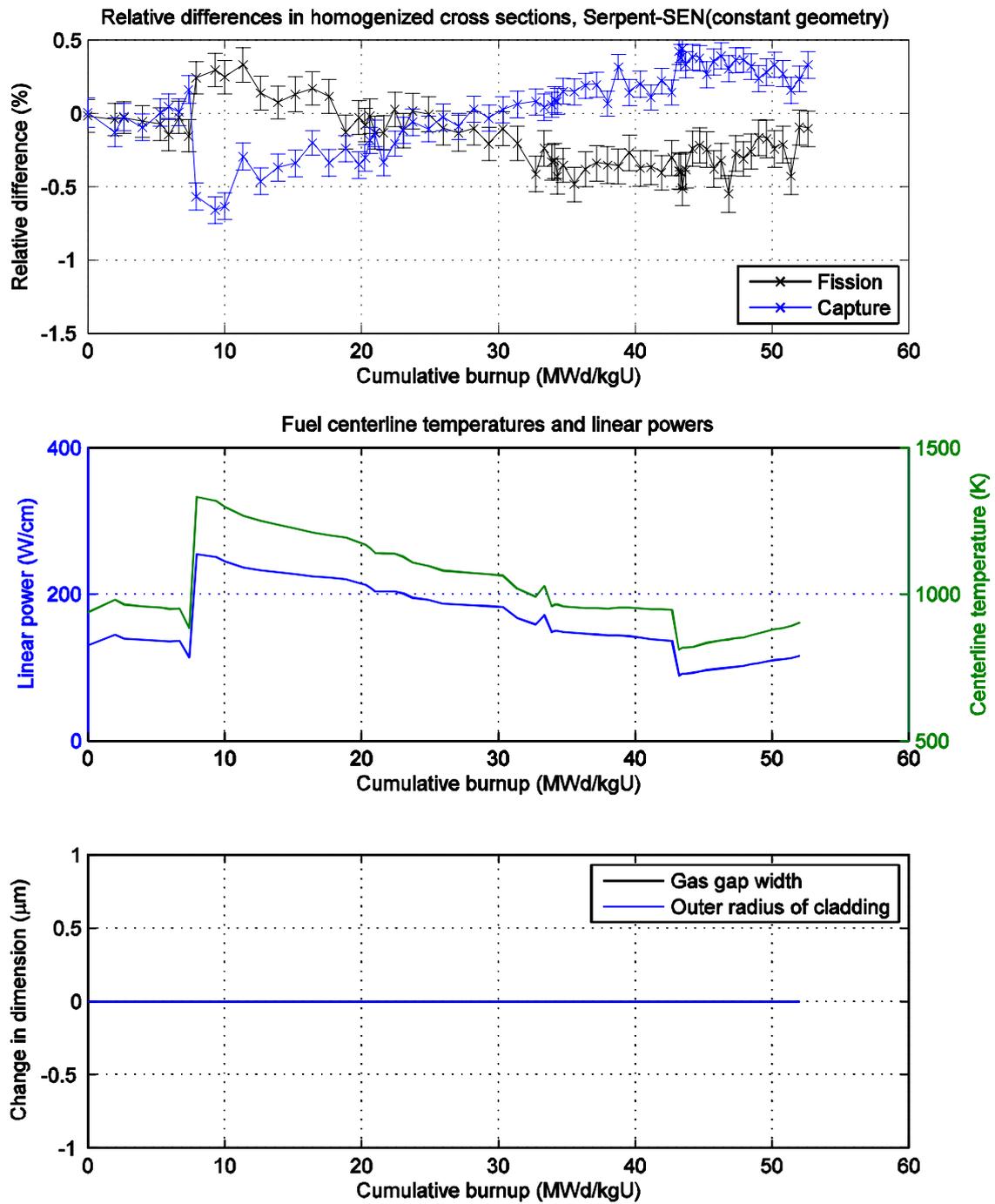


Figure 8: Results of a special SEN simulation in which the geometry was kept constant and only temperature was varied. High linear power case.