Ville Rintala

COUPLING MONTE CARLO NEUTRONICS WITH THERMAL HYDRAULICS AND FUEL THERMO-MECHANICS

ACTA UNIVERSITATIS LAPPEENRANTAENSIS 1059

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Supervisors Professor Juhani Hyvärinen
LUT School of Energy Systems
Lappeenranta-Lahti University of Technology LUT
Finland

Post-Doctoral Researcher Heikki Suikkanen
LUT School of Energy Systems
Lappeenranta-Lahti University of Technology LUT
Finland

Reviewers Professor Christophe Demazière
Department of Physics
Chalmers University of Technology
Sweden

Researcher Stefano Lorenzi
Department of Energy
Politecnico di Milano
Italy

Opponent Dr. Sören Kliem
Nuclear Safety
Helmholtz-Zentrum Dresden-Rossendorf
Germany

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Abstract

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Coupling Monte Carlo neutronics with thermal hydraulics and fuel thermo-mechanics

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This work aims to improve the coupled calculations required for the modeling of nuclear reactors by producing more advanced computational tools.

The study applies more advanced computational tools to more detailed modeling of the random structure in pebble bed reactors and temperature distributions formed in the fuel rods of light water reactors. As part of the calculation applied to light water reactors, a coupling code is created that links the reactor physics code utilizing the Monte Carlo method and the traditional fuel code to the coupled calculation.

The calculations performed in pebble bed and light water reactors show that the Monte Carlo reactor physics code can be used as part of a calculation system that produces accurate comparison results or solves specific challenging problems where increased use of calculation capacity is justified. The comparison results calculated by such a coupling can be utilized in the future to improve the accuracy of simpler and faster calculation codes.

Keywords: Monte Carlo method, neutronics, thermal hydraulics, fuel behavior

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Research is almost always teamwork and I am lucky to have such a research colleague as Heikki Suikkanen is. He has taken care of many complicated tasks in our research on those fields which are more unfamiliar for me. I want to thank you for all your help over the years which we have been working together.

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Jaakko Leppänen has developed a great Monte Carlo reactor physics code Serpent which has been used in this work extensively. Jaakko developed a randomly packed pebble bed model in Serpent to address our problem to solve power distribution in such geometries. Thank you for the support with Serpent and also for taking care of a part of the teaching of reactor physics courses in LUT.

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Ville Rintala
October 2022
Lappeenranta, Finland

Contents

List of publications

This thesis consists of an introductory part, three original, refereed articles in scientific journals and one original, refereed conference article. The articles and the author's contribution to them are summarized below.

I **Rintala V., Suikkanen H., Leppänen J. and Kyrki-Rajamäki R.**. Modeling of realistic pebble bed reactor geometries using the Serpent Monte Carlo code, *Annals of Nuclear Energy*, 77, pp. 223-230, 2015.

II **Suikkanen H., Rintala V., and Kyrki-Rajamäki R.**. Development of a coupled multi-physics code system for pebble bed reactor core modeling, *7th International Topical Meeting on High Temperature Reactor Technology (HTR2014)*, Weihai, China, October 27-31, 2014.

III **Suikkanen H., Rintala V., Schubert A. and Van Uffelen P.**. Development of coupled neutronics and fuel performance analysis capabilities between Serpent and TRANSURANUS, *Nuclear Engineering and Design*, 359, 110450, 2020.

IV **Rintala V., Suikkanen H., Schubert A. and Van Uffelen P.**. Supplementing fuel behaviour analyses via coupled Monte Carlo neutronics and fission product solution, *Nuclear Engineering and Design*, 389, 111668, 2022.

Author's contribution

The author is the principal author of Publication I and Publication IV and has participated in writing Publication II and Publication III. In Publication I, author has created reactor models and done related computations. In Publication II, the author has generated reactor physics calculation models and analysed power distribution related calculation results and in Publication III, the author has written coupling script taking care of calculation process. In Publication IV, the author has developed the coupling script to transfer the nuclide data between the reactor physics and the fuel behavior solvers.

CHAPTER 1

Introduction

Nuclear power plants typically produce a lot of energy with low emissions, and the production of power is very predictable. The energy content of fuel is high, yet the amount of nuclear fuel required is small, which means that fuel costs represent a small part of the total operating costs of a nuclear power plant.

However, the price of a single fuel bundle is calculated in hundreds of thousands of euros; hence, the use of fuel should be optimized, despite being a small share of the total costs. On top of the stresses occurring in normal use, nuclear fuel must withstand the additional stresses caused by possible accident scenarios. One of the fundamental safety functions [1], the confinement of radioactive material, where fuel cladding acts as the first barrier, aims for the cladding to remain intact. To answer most of the questions related to the integrity of nuclear fuel, conditions in the fuel must be modeled throughout the operating life of the fuel.

Of particular interest are the fuel power distribution, temperature distribution, nuclide distribution and their evolution as a function of time, as these dictate the thermal and mechanical response of the fuel to reactor operating conditions, normal or abnormal. Power and temperature distributions are driven by the neutron distribution in the reactor, which in turn is affected by the fuel temperature and composition, therefore a coupled solution of the neutronics, heat transfer and fuel burnup is necessary.

Nuclear fuel-related computations are typically performed in a two-step process, in which the volume formed by the cross-section of a single bundle and the appropriate height range is first homogenized using neutron transport theory. This calculation is repeated for different fuel bundle types under different physical conditions; these are used as the building blocks in the second step of calculation process, at which point the core-level problem is solved.[2] The Monte Carlo method can be used as an alternative to deterministic neutron transport solvers in the generation of group constants at bundle level calculations[3].

The core solution is most often based on a computational code using the diffusion

equation, which solves the reactor multiplication factor and power distribution over the operating cycle. Utilizing the results obtained in the homogenization, the information obtained in second step can be transferred back to the rod level and, thus, help in calculating for example, the accumulation of burn-up in the fuel.[4]

These data can be further applied as an input to analyze individual fuel rod modeling to determine nuclear fuel behavior during normal operations and possible accident conditions.

These methods work in and of themselves, but different assumptions are made throughout the calculation chain. In addition, the calculating system is never perfect. There is always some uncertainty in the final result, and to reduce this, on the one hand, measurements are needed for comparison. On the other hand, better calculation methods are needed to replace less-accurate solutions or for comparisons to understand how to improve the solution.

In the field of reactor physics, Monte Carlo–type solution methods allow such development work because they need to have a smaller number of assumptions when solving reactor problems. This should lead to more accurate calculation results or, at the very least, reveal normally latent, possibly overlapping, different kinds of errors.

The disadvantage of Monte Carlo methods is the high computing power requirements, which have eased significantly over the past 10 years with the general development of computers, which have made it possible to exploit Monte Carlo methods in new applications.

Pebble bed reactors

In pebble bed reactors, the spherical fuel elements with fuel particles inside them form a random structure on two levels. The random placement of the fuel pebbles causes difficulties in performing homogenization because the structure of the core cannot be divided into constantly repeating sections.

Pebble beds have been subjected to various simplified studies in which the positions of fuel pebbles are arranged in a regular structure. By varying the distance between pebbles, a packing density of the bed can be changed; here, the aim is to make this the same as the average packing density of the reactor. However, this does not accurately model the structure of the pebble bed because the shape of the reactor affects the placement of the pebbles and a variation in the packing density is expected in real-life cases.

On the other hand, the fuel particles in each pebble are randomly distributed, and in many modelings, the particles are also placed in some kind of constant

lattice. For example Difilippo has modeled pebble bed using pebbles and individual fuel particles in case of PROTEUS facility [5]. In some cases, both the fuel particles and fuel pebbles are not intersected in a physically correct way at the boundary surfaces. Brown and Martin have introduced randomness to the modeling of fuel particles within MCNP5 Monte Carlo code [6]. MONK Monte Carlo code uses Woodcock tracking method and has the possibility to model individual pebbles and particles in an explicit way. A simplified method for creating a random placement of pebbles has been developed too[7].

Light water reactors

In detailed calculations of light water reactors, emphasis has been placed on various multiphysics applications that are using a state-of-the-art approach in at least one specific solver. The aim is to perform the calculation with a more accurate solution method and improve the understanding of the phenomena, as well as to produce results for comparison with less accurate but faster solution methods.

In typical cases, the solution for reactor power distributions works reliably, but major changes in fuel composition, such as inserting burnable poison or using accident tolerant fuels, can cause uncertainties in the results. For example, in such situations, there is a need for more specific methods that can be used as reference cases.

One multiphysics application is to accurately calculate the power distribution of fuel at the rod level with the Monte Carlo code and use this in a fuel code, in which an accurate internal power distribution within the rod is especially useful.

Work related to high-fidelity modeling and multiphysics include efforts done in projects such as the European NURESIM platform [8], the MOOSE simulation environment at the Idaho National Laboratory [9] or the work within the CASL consortium established by the US Department of Energy [10]. These are frameworks including a vast amount of different solvers to different purposes. More recent developments include KRAKEN framework developed in VTT [11]. In addition to these, more modest contributions have been done by others where some specific solvers have been coupled to obtain detailed high fidelity solution. Valtavirta has worked on to develope multiphysics interface in Serpent Monte Carlo code to include possibility to use Monte Carlo solution with fuel behavior solvers [12]. Valtavirta et al. have coupled Serpent with fuel performance codes ENIGMA and Finix with this developed interface [13]. Serpent has been coupled with subchannel thermal-hydraulic and fuel behaviour solvers by García et al.[14]. The work by García et al. shares similar tools as used in this work but their main focus has been on core-level calculations.

1.1 Objective of the study

In the current work, the accuracy of calculation methods in solving complex practical problems is developed. The work shows that reactor physics calculations using the Monte Carlo method can be used as part of a coupled calculation and can be done with reasonable effort.

The advantages of the Monte Carlo calculation system are studied in two different cases: coupled calculations in pebble bed reactors and light water reactors. The objectives of the present study are as follows:

- To model the random double heterogeneous structure of pebble bed reactors more accurately than traditional computational tools have been able to.
- To investigate the solution of the power distribution of the pebble bed reactor using the Monte Carlo method, here taking into account the random structure of the pebble bed and random placement of fuel particles. In addition, an aim is to see whether a solution based on such an approach can be used as part of a coupled calculation for an entire reactor.
- To develop a coupling code using a traditional fuel thermo-mechanical solver and Monte Carlo reactor physics solution for analyses of a light water reactor fuel.
- To assess if such coupling can be applied to study practical problems with current computer capacity. If yes, could the results be used as references for more traditional calculation tools?
- To investigate if the burn-up modeling capabilities of Monte Carlo reactor physics codes can be used to produce nuclide concentrations for coupling with reasonable effort instead of using less-accurate methods provided by fuel codes.

1.2 Research methods

The current research uses computational tools that have been found to work properly when used in their own application area; these are used to form interoperable coupled solvers. The research material is the calculation results produced by the coupled solvers, which are interpreted to find out the answers to the research questions. The research is empirical, and the research method is the collection and observation of calculation results based entirely on quantitative methods.

For cost reasons, it would be impossible to elucidate the issues examined in this work by making actual measurements. Such experimental arrangements will be replaced by computational analyses performed with computational codes previously demonstrated to be effective in experiments performed by others. The work assumes that the calculation tools used will work well enough in their usual application range and produce reliable results based on the given input data.

1.3 Description of content

This is an article-based dissertation with a summary section and research articles attached to it. The first chapter of the summary section describes the research topic in general and the basic idea behind the research. The second chapter reviews theories needed to understand the work and how the current study is related to previous research. The third chapter describes the research process and results obtained from it. The fourth chapter answers the research questions based on the results while considering their significance. The fifth chapter presents the main conclusions of the study.

CHAPTER 2

Coupling of Monte Carlo reactor physics

The aim of the study has been to model things more accurately than has previously been possible. The constraints are largely due to the availability of computing power, which has further limited the available computational methods. Typically, the calculation is performed as described in the theoretical chapter by dividing the calculation into parts and solving a simplified problem for the whole reactor by using homogenized geometry. Most of the practical calculation work at nuclear power plants is done with deterministic calculation codes. The advantages of these deterministic calculation codes are the speed of the solution and the constant accuracy of the solution according to pre-selected choices. The disadvantages are these same choices, which, on the other hand, achieve sufficient accuracy at a reasonable speed. With deterministic methods one has to make some assumptions, such as discrete directions and energy, and this inevitably affects the computational accuracy.

The Monte Carlo method is based on tracking of a single neutron at a time, so several assumptions can be overcome, such as the directional and energy discretions described above. Thus, by using the Monte Carlo method, significantly fewer assumptions can be made and by solving the same problem with the same initial values, the results should be more accurate calculated by the Monte Carlo method compared to deterministic methods. A single neutron history does not tell much about the behavior of the reactor, so a very large number of neutron histories must be calculated. The problem here is, obviously, the considerable need for computing power, and for this reason the practical applications have been quite limited, with some exceptions.

However, modern computers and high performance computing systems built from them, have made it possible to apply the Monte Carlo method to completely new problems in reactor physics, and in this study it is being applied to the calculation of power distributions in pebble bed reactors and light water reactor fuel rods.

The behavior of nuclear reactors is generally well known and this knowledge is

based on theoretical laws, previous operating experience and experimental research. However, going to the detailed level, the results are affected by a variety of uncertainties, or some kind of model is used in the calculation, which evaluates, for example, the average behavior of a large set of neutrons without actually modeling the detailed behavior. This means that the deterministic methods used are usually limited to a pre-determined range of applicability, and deviating from this may require significant changes to these methods in order to achieve sufficient accuracy. Most often deterministic calculation tools are made to be used for one reactor type, such as an light water reactor, and even using hexagonal fuel instead of rectangular might need a special version of software.

Using the Monte Carlo method, the same calculation tool can be used in very different situations, as there are very few assumptions required. The computational accuracy should also be better with similar initial values when compared to deterministic codes, and thus the Monte Carlo solution can be used as a kind of reference point to study the accuracy of commonly used deterministic, much faster computational tools.

2.1 Monte Carlo method

The calculation code using the Monte Carlo method gives results for some predetermined volumes and this division can be similar with the geometry model or with structures described as completely different. If the volumes are very small, they will be hit by few neutrons and the statistical uncertainty will increase. If, on the other hand, these volumes are increased, then the phenomena occurring in a certain place can no longer be monitored, i.e. the spatial resolution is inaccurate. Results collected within a single detector volume are typically constant. Another option is to use function expansion tallies (FET) [15], which are function expansions that can be adapted to the reaction distribution. These aim to avoid problems with constant values and in some ways this has similarities to the idea behind nodal diffusion. One kind of intermediate form of these is to fit a suitable function to the results, which then describes the form of the results.

The statistical accuracy follows the neutron density or reaction rate distribution and this depends on the type of detector used to record results. Events that produce statistics are proportional to the above-mentioned variables, and the spatial resolution of the results can be more accurate, for example in high power areas. Correspondingly areas with less reactions like, for example, near reactor edge, the spatial resolution must be coarser to collect enough results to get acceptable statistical accuracy.

2.2 Coupling of Monte Carlo reactor physics in pebble bed reactors

2.2.1 Discrete Element Method

Pebble bed reactors consist of a large number of randomly distributed spherical fuel elements, and when modeling such a bed, its structure must be known in order to develop a model or calculation method which describes average behavior of such bed. Efforts have been made to model the structure of the bed in many ways, but the discrete element method (DEM) method is likely to provide a computational solution to the problem that is closest to the real case currently[16]. Here, contact forces affecting each pebble are taken into account, position of each fuel pebble is solved and the random pebble bed formed in the reactor can be solved by starting from some known initial configuration. In practice, this is a randomly packed structure, and the DEM method seeks to find a structure that sufficiently mimics a real pebble bed. A better computational solution would be obtained mainly with methods based on strength calculations which are using something like finite element method.

Heikki Suikkanen has packed the fuel pebbles of pebble bed reactors with DEM calculation, and more information about packing can be found from his dissertation [17], sections related to packing in Publication I, Publication II and article [16]. Packing calculations have been made with unnamed in-house DEM code of LUT, the Esys particle[18] and for the most part with the LIGGGHTS[19] code.

The aim of packing is to obtain a result in which the packing density and its distribution mimic the situation in the actual reactor. By randomly drawing locations, this is not possible. There is a limit in the packing density that pebbles cannot exceed by randomly drawing positions. This is easily understood by thinking that pebbles are drawn into empty space and pebbles are positioned randomly. If a pebble placed in a drawn position overlaps with an existing pebble, the position is discarded and the draw is performed again. Adding pebbles eventually results in a situation where the voids between the pebbles are filled and the pebbles can no longer be placed in the gaps. However, there is still some empty space between the pebbles and the packing density achieved is limited. Without a better method, denser packing densities can only be achieved with a regular structure, which in turn does not accurately describe the structure in principal level.

When calculating with the DEM, it may not be advisable to use actual material properties, as their effect on the final result may be small, but the calculation time may be multiplied manyfold. In practice, packing calculations have some kind of initial situation in which the pebbles are drawn into a sparse structure, into

which they are obtained by random packing as described above, and the pebbles are allowed to fall into a reactor-shaped calculation model. Once the pebbles are in place, it is examined that the structure of the pebble bed complies with the desired conditions. These conditions can be, for example, the height of the bed and packing density distribution. If the bed is too sparse, the bed can be shaken to make the pebbles pack in denser structure. There are many challenges associated with packing, and if very realistic packing process is simulated, computing power requirements can also increase significantly.

Once the pebble bed is formed, the locations of all the pebbles are given from the DEM code as coordinates in result files and these can be placed in the MC model by using the pbed structure of Serpent. Here, in addition to the position coordinates, the radius and type of the fuel pebble are given.

DEM code produces the location information of the fuel pebbles and the resulting single packing can be used in the reactor physics calculation to describe pebble bed at one point in time. This is often sufficient because, in many computational cases, omitting modeling of time dependence does not lead to problems as changes are slow. For example, burnup of nuclear fuel will not change significantly in the short term and it is not necessary to take such a change into account. It is trusted that small changes are not changing local phenomena significantly.

2.2.2 Thermal hydraulics

A general-purpose CFD code was used for the thermal hydraulics and the thermal hydraulic model was made by Heikki Suikkanen and more detailed information related to thermal hydraulics can be found in his dissertation [17]. The calculations were performed with Ansys Fluent code where the porosity model was used for modeling. When calculating with the porosity model, a solid substance is used in the calculation cells, through which the flow can still pass. The flow resistance is determined based on the porosity value entered into each calculation cell. With the exception of the porosity model, thermal hydraulic calculations require so much computational power that the use of any other, more precise, method is not yet possible, at least for some time, in the calculation of the entire reactor. Only possible exceptions could be exascale level supercomputer analyses and even then, used geometries are somewhat limited.

The porosity values for the calculation cells of the thermal hydraulic model were calculated from location information given by DEM code and mesh cell boundaries used in the porosity model. A structural type mesh was used for the calculation cell division, aiming to hold at least 10 fuel pebbles in each calculation cell. On the other hand, the size of the calculation cells should be small enough so that the resolution of the thermal-hydraulic calculation model is appropriate.

The pebbles were divided into calculation cells according to their actual surface areas, as the placement based on the center points was already found to be too inaccurate. This was due to existence of some repeating structure in positions of the fuel pebbles, which may lead to repeated fluctuations in the number of fuel pebbles inside calculation cells. Even if the pebbles are placed randomly in the reactor core, if the location of one of the pebbles is known, then the location of nearby pebbles at certain points is more likely and predictable due to the same size of the pebbles and the way they fit together in the core. In practice, there is more pebbles in every second calculation cell and less in cells between. This, if pebbles are positioned to calculation cells by center points, leads to repeated fluctuations in porosity and power values given as input for thermal hydraulics. The main reason for this phenomenon to occur is the radii of the fuel pebbles being of the same order of magnitude as the dimensions of the calculation cells.

Based on the reactor physics calculation, thermal power data was entered into each calculation cell in the thermal hydraulic calculation, and as a result from calculation, fluid temperature and surface temperature of the solid part of the porous material, are obtained. These can be again used in reactor physics calculation.

2.2.3 Reactor physics

Serpent Monte Carlo reactor physics code developed in VTT [20] was used for calculations. The Serpent model of the pebble bed reactor roughly consists of the reactor structures and the pebble bed acting as the reactor core. The structures are modeled by forming all the necessary delimiting surfaces and these surfaces are then used to delimit cells which can be actual components such as reflector or empty spaces in the reflector. Likewise, control rods, instrumentation tubes and all other desired structures are assembled by using surfaces and cells. The region of the reactor core is filled with a pebble bed universe for which pebble location information was obtained using a DEM code.

The pebble bed of the reactor core is, at this stage, made of fuel pebbles without any specific structure defined. In addition, a background universe has been defined in the region containing the pebble bed, which is simply helium acting as a coolant. To determine the structure of the pebbles, different fuel pebble universes are created for different pebbles and the most suitable option is selected for each pebble. This feature can be used to select different fuel particle distributions for the pebbles, or it can be used to select a fuel pebble with a specific temperature for specific location from different options available.

There is a similar random packing problem inside fuel pebbles as in the pebble bed itself, because the particles in the fuel area of the pebble are randomly dis-

tributed. Now the problem is bit easier to handle as packing density is so low that fuel particles can be drawn into suitable locations without the use of the discrete element method. In Serpent, the same geometry type can be used to describe the particles in the fuel pebble as was used to describe the pebble bed in the core. Here graphite acts as the background universe and the temperature of graphite can be defined in several ways. It is desired to determine the temperature distribution of graphite because graphite is abundant in the core region and its temperature has an effect on reactivity. The temperature of the graphite increases towards the center of each pebble and this can be calculated by using one-dimensional thermal conduction equation. Alternatives from the perspective of a single pebble include some kind of average temperature or division into several layers that tend to model the temperature distribution of graphite. Similarly, universes can be defined individually for particles, and this allows different temperatures to be taken into account by taking certain particles to a certain depth in the fuel pebble. In fact, the temperature is determined by the material used and the material can be Doppler broadened to a suitable temperature at the beginning of the calculation. Each nuclide in different temperature consumes memory on the computing servers, which limits the number of temperatures that can be used. This is particularly problematic in burnup calculation cases. Serpent 1 was used in pebble bed reactor calculations and some limitations are related to the version used.

The pebble bed model in Serpent enables fission power to be calculated in pebble-wise manner, i.e. the detector structure is automatically formed to pebble bed and the resulting thermal power information can be written to a file. Furthermore, the power information is distributed to the calculation cells in relation to the surface area exposed in them, i.e. the right amount of power ends up in each calculation cell, and then the data should be correct from the viewpoint of the porosity model.

The actual coupled calculation is started by assuming some kind of temperature distribution in the reactor and this is used in Serpent to calculate power distribution. The calculated power distribution is fed into Fluent and new temperatures are obtained.

2.2.4 Detailed modeling of randomly packed pebble bed

Availability of measurement data for randomly packed pebble bed reactors is quite limited. One of the cases is the ASTRA criticality benchmark of the Kurchatov Institute [21]. In this experiment criticality with five different bed heights are studied and associated control rod height positions are searched. Quite comprehensive documentation of the experiment is available from the OECD NEA databank, and it was decided to use this case as a test case for a random pebble

bed.

The ASTRA criticality facility consists of graphite blocks used as reflectors at the bottom, sides and center of the reactor cavity. Control rods are placed in the holes in the blocks at specific positions. One control rod and its guide tube are located in the middle of the annular pebble bed, as are a few instrumentation tubes.

The starting point was to pack the pebble bed in the core area as realistically as possible, and in fact the only major simplification was to exclude the support structure of the control rod tube located on the bottom of the core from the DEM model. The effect of this simplification as being a local structure was estimated to be very small and the same assumption was used in the reactor physical model.

In the reactor physical model, the fuel pebbles were defined very precisely and placed on locations given by the discrete element method. The fuel particles in the pebbles were randomly placed by creating particle distributions in advance. A limited number were used and in this case 10 different fuel particle distributions were considered to be enough. Jaakko Leppänen developed a model for Serpent that is suitable for describing a pebble bed reactor, and this was taken into use in the pebble bed reactor model.

The different calculation cases were solved using proper bed height and the positions of the control rods as given in the documentation for each case. An example of packing of a pebble bed is shown in figure 2.1. Before reviewing the results, a variety of non-modeled factors and effects of assumptions should be considered that may cause discrepancies in the results.

The detailed modeling of pebble bed reactor core is presented in Publication I. Most important results are given in Section 3.1.

2.2.5 Random packing with coolant thermal hydraulics

The calculation of the random pebble bed was continued in an effort to solve the reactor power distribution at the level of a single fuel ball and to utilize this power information on the thermal hydraulics solver. A simplified case simulating a HTR-PM reactor with a cylindrical core region and a funnel-like structure at the bottom was chosen as the model. In this case, a pebble bed consisting of 430 000 fuel balls was formed using discrete element method.

In addition to the pebble bed in the core area, the reactor physical model consists of a reflective graphite and pressure vessel made from steel. The lower part of the reactor has a funnel structure similar to that of the HTR-PM. The fuel pebbles were modeled in the same way as in the case of ASTRA, i.e. a limited number of random distributions were formed in advance for the fuel particles and

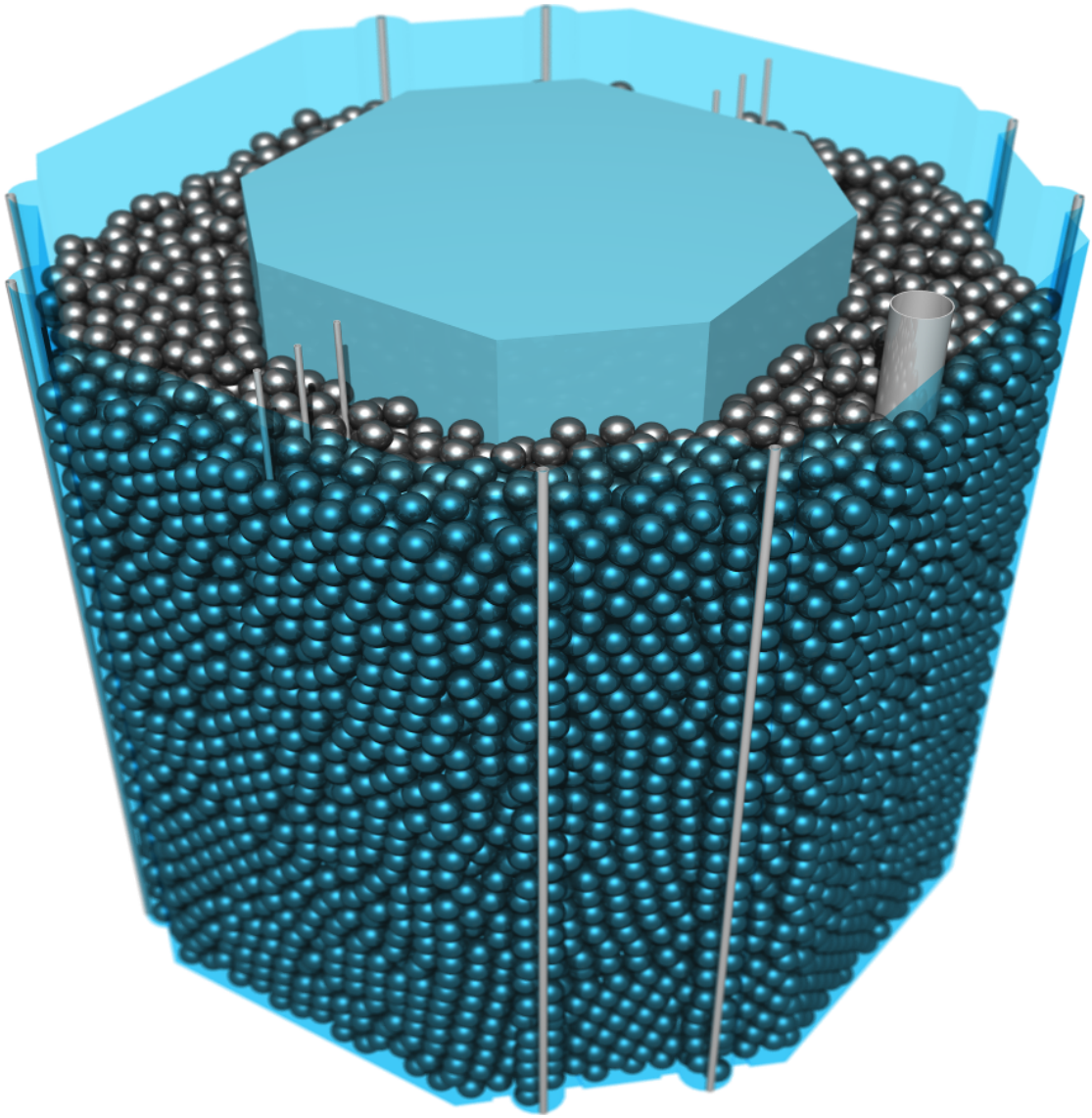

Figure 2.1: Pebble bed corresponding to ASTRA core configuration 1 with 16 897 pebbles constructed using DEM.

these were used to randomly place the particles into pebbles. In addition, the effect of temperature on reactivity was taken into account more accurately by making a layered structure to pebbles in which the materials have different temperatures. Calculations were performed with Serpent 1.x versions. The Serpent tmp card was used to supply the temperatures, allowing materials to be Doppler broadened to desired temperature before starting the actual calculation. Temperatures in pebbles were calculated simply by using 1D heat transfer equation with assumed effective thermal conductivity in the radial direction of the fuel pebble. Next, the temperature profile for each pebble could be calculated and the

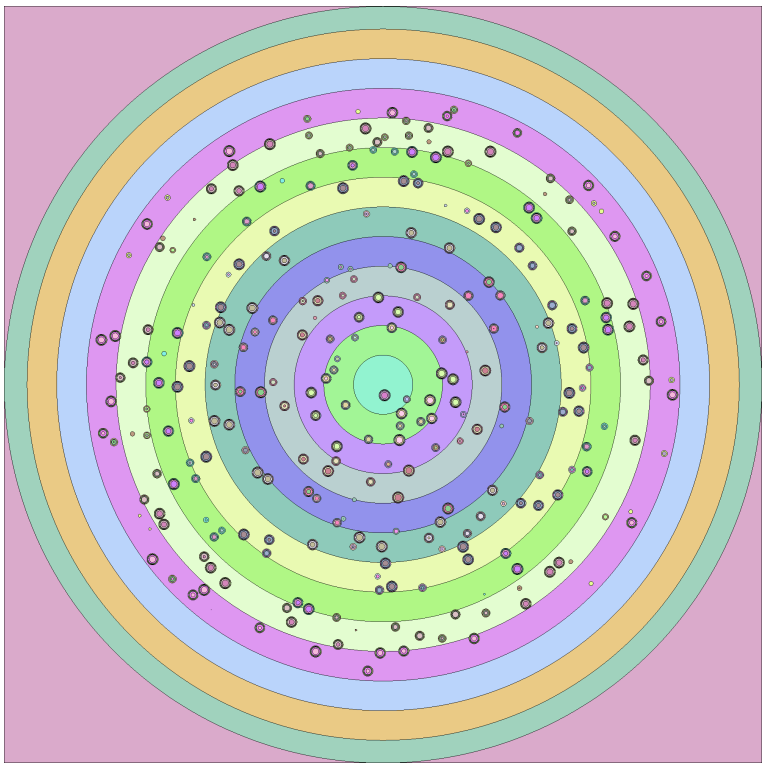

Figure 2.2: Cross section of a fuel pebble model in Serpent with coupled thermal hydraulics. The pebble is divided into several layers for which different temperatures are assigned.

temperature of uranium oxide in the fuel particles could be estimated by similar methods.

Amount of different temperature values were limited by available computer memory as each doppler broadened material requires its own copy of nuclear data. Figure 2.2 shows the temperature division in which the fuel pebble is divided into 13 layers. There are 10 layers in the fuel area and 3 in the surrounding graphite. Temperatures were determined starting from the surface temperature of porous material which was given by the porous solver of the computational fluid dynamics code.

ANSYS Fluent was used as the thermal-hydraulic solver, and the pebble bed was modeled using a porosity model, because otherwise the computational power requirement would have been completely impossible from the point of view of the computational resources available for the task. The material is thus assumed to be porous, and the temperature of the helium acting as a coolant and the surface temperature of the fuel pebbles, which are acting as the porous material, are obtained from the thermal-hydraulic solver. The calculation cells had to be large

enough to contain enough particles so that the porosity model remained a valid approach. In this calculation, care was taken to ensure that there were at least 10 fuel pebbles in each cell, and if this was not the case, the porosity was calculated by taking average of neighboring cells.

The calculation was started with a constant temperature distribution in Serpent and the power distribution produced was transferred to Fluent by collecting the necessary results with the help of scripts. In the thermal-hydraulic solver, the new temperatures were calculated for the surface temperature of the fuel and based on these, the temperatures present in the fuel were estimated. Based on these temperatures, temperatures for materials to be Doppler-broadened were selected and the Serpent input file was written for the next iteration. The temperatures of the fuel particles and graphite were set in the Serpent input file and this information was used to describe fuel pebbles having different temperatures. In the pebble bed input file, the selection was made where pebbles having some specific temperature were actually positioned. The effect of helium as a coolant was not accurately modeled in the reactor physics solution due to its estimated low importance.

Pebble bed reactor coupled calculation with Serpent and Ansys Fluent is presented in Publication II. Most important results are presented in Section 3.2.

2.3 Fuel behavior coupling in LWRs

In fuel code coupling, the basic idea has been to improve the reactor physics solution in traditional fuel codes. The traditional fuel codes are 1.5-dimensional, meaning that the actual modeling takes place in the radial direction of the fuel rod and in the axial direction the fuel rod is divided into a sufficient number of sections in which the calculation is repeated. The calculation of the axial sections of the fuel depends on each other through the gas gap, because the gas gap of the rod is common to all axial sections. In principle, the fuel code knows nothing about neighboring rods. Furthermore, this means that the reactor physics solution of the fuel code is made of a fuel modeled in a infinite lattice. This may or may not be a good solution depending on the case being modeled. An example of an unfavorable situation is rods containing burnable poison. Such rods are not evenly distributed in the fuel bundle, but are only a few of the bundle rods. Modeling a rod containing a burnable poison in infinitely repetitive geometry clearly does not accurately describe the situation. Because of this, special models have been added to the fuel behavior codes in an effort to correct the problem. In principle, such fixes tend to have a limited scope and this makes it difficult to apply codes to new problems.

The problem itself is well known and as part of the development of the VVER-440 fuel in the ESSANUF EU project, it was decided to try to fix the issue with regard to the TRANSURANUS code [22]. There was a desire to use a more accurate method that could be used to produce the most accurate power distribution possible at pin level. These accurate results could be used directly to solve the fuel behavior problem with the fuel code if the elapsed computation time was justified to obtain such more accurate result, or these results could be used as a reference when using or developing faster deterministic reactor physics solvers.

2.3.1 Main features of coupling

There is always some sort of problem in the coupled calculation at start-up, as the initial power and temperature estimates should be as good as possible. This minimizes the necessary iteration rounds. In practice, the coupling requires power information for the fuel code in each axial section and its radial distribution. Correspondingly, temperatures are required for the reactor physics solver in all modeled reactor sections. The most important temperature information is from reactor physics point of view, in the fuel and, in the case of light water reactors, in the moderator.

Of course, a coupled reactor physics solution using Monte Carlo solver is not a good alternative to the calculation of the whole core of traditional reactor due to the computational power requirements. Only a smaller area can be solved at least if the radial power distribution of each rod is to be taken into account. In practice, this is an area to be solved with a few rods, one bundle, or a maximum of some bundles without a large scale computer cluster or supercomputer.

The conditions of the area of interest must be made to resemble the real case, and yet for computational reasons, reflective boundary conditions have to be used. For this reason, the surroundings of the region of interest should be modeled from a sufficiently large area to avoid distortion of the neutron flux. Determining the size of the area to be modeled is case-specific. This does not describe the situation completely correctly, but is in any case much better than the single rod model of the fuel code can be.

The solution requires some kind of normalization condition, which in the case of a reactor physics solution is most often the thermal power produced in the area. In practice, this is obtained from a deterministic whole core computation like a core simulator.

In the case of a fuel behavior code, the boundary condition is the temperature of the water cooling the fuel and the heat transfer coefficient from which the surface temperature of the fuel rod can be determined, as long as the material properties

and the power released in the rod are known. At this point, it is good to note that there is no solution for the coolant temperatures involved in the coupling, i.e. these are assumed to be known. Again, this information is available from the core simulator.

When starting a solution, it is worth considering which source data is the most reliable and produces the best data to be transferred first. Another thing to consider is the time it takes to solve, in which case the fastest solver should usually be used first to give the slower solver better data than the initial guess. The reactor physics solution should know the fuel temperature in the different parts of the rod and for the fuel behavior the power, respectively. It was decided to solve the problem by using the fuel behavior code at the beginning of the calculation to solve the power and temperatures independently, i.e. it was used in the traditional way.

This so-called zeroth iteration yielded a temperature distribution in the fuel, which was transferred to the Serpent and the first more correct shaped radial power distribution was solved. Next power distribution was transferred to the TRANSURANUS code and better temperature values were solved.

Coupling approaches can be divided to segregated and monolithic. In segregated approaches different mono-physics are coupled together and monolithic where whole multi-physics problem is solved by a single solver. [23] In this coupling separate solvers were used for the mono-physics and segregated approach was the only option.

2.3.2 Coupling code

There are several options for implementing the coupling data transfer, one being input/output file approach and other relying using common shared library in one form or other. These options include compiling solvers into a single executable or using library like message passing interface.[23]

Both calculation codes use input files in ASCII format and eventually produce ASCII output data. Input/output file approach was chosen for coupling because of overall simplicity and to avoid modifying the software used. In an alternative shared library approach, data would have to be collected from variables while the software is running and then transferred from one program to another using a common shared library. This would mean creating this shared library and incorporating it with the necessary routines into both software. The biggest problem would probably be that this code would have to be maintained as the software is changing and this could easily cause problems for all parties. The Monte Carlo solution was also known to be slow and the deceleration caused by the

input/output file approach is not a significant part of the total computation time.

The coupling code was implemented in the Perl programming language and the main reason for using Perl was the ready-made routines suitable for processing data in text format. In addition, some suitable scripts were done in Perl earlier and there was no desire to rewrite them in another programming language. Python was mainly considered as an alternative, but with many other software languages, it is more difficult to process such text data without using additional libraries.

In the version of the coupling code used in this work, the coolant temperature was not solved in the calculation, but was given in advance as a boundary condition. In practice, this produces error in the calculation if the axial power distribution, which the temperature solution is based on, does not correspond in shape to that calculated in the coupling.

Figure 2.3 shows a flowchart of operation of the coupling code. The calculation is started from the initial state presented by input files of the coupling code and involved solvers and ends with the last burnup step given.

The coupling code starts the calculation by collecting necessary input data from its own input file and creates calculation code specific input files from templates. Coupling script adds calculation-specific data relevant to the coupling in these inputs. Initially, in the first burnup step, the coupling code runs TRANSURANUS code in standalone mode to form a better initial guess. The coupling then proceeds to the actual coupling loop.

The previous TRANSURANUS results are read first in the coupling loop and then Serpent is run for the entire geometry. On Serpent side, a fuel behavior coupling interface written by Valtavirta et al.[13] is used. Serpent is started in the background at the beginning of the calculation and the calculation process between the coupling code and Serpent is controlled by POSIX signals according to the operation of the fuel interface. After Serpent resolves a new power data, it is left in the background waiting for the next iteration. The results are read from Serpent output file and the coupling code processes new TRANSURANUS code input files using the power data. This is done by first collecting axial power data and then solving relative values for radial power data. After this processing the data is being appended to TRANSURANUS input file templates and then TRANSURANUS is run on each coupled rod separately.

Each burnup step is iterated by solving the power distribution and fuel temperatures turn-by-turn until the cut-off condition is reached. At the end of the current burnup step, the fuel code is used to calculate the final temperatures for the iteration. Then the coupling script moves on to the next burnup step and final temperatures are used as initial values for power solution of the next burnup

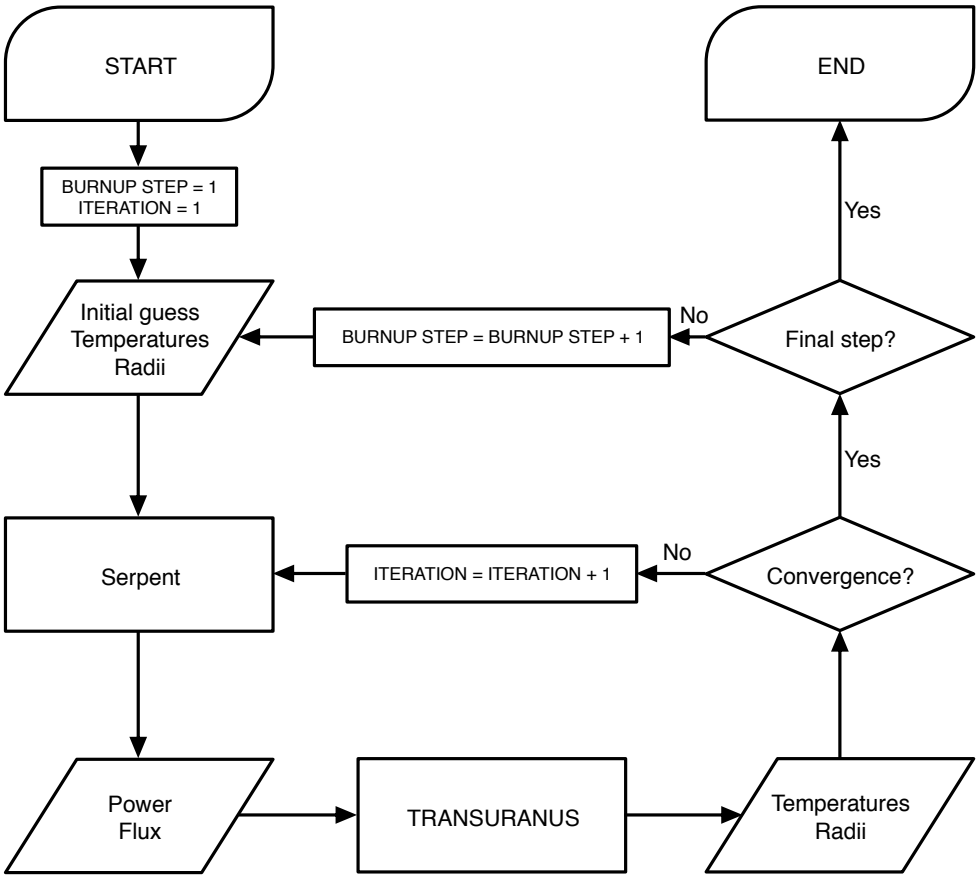

Figure 2.3: Flowchart of a coupled Serpent - TRANSURANUS calculation.

step. The process repeats until the last burnup step ends the computing.

2.3.3 Monte Carlo computed power distribution in fuel pins

The results of a Monte Carlo-type reactor physics calculation are typically reaction rates at defined volumes. The fuel code uses calculation points where values are calculated and different initial values must be known. For example, power distribution is given for such points, so the results given for volumes by Monte Carlo code must be converted to a point-like format.

TRANSURANUS needs the power profile in the axial direction and in addition a

value describing the power profile for each calculation point of each axial section. The coupling code must be able to perform the conversion between data formats. This is done by taking the midpoints of the volumes and setting straight lines between them. This is illustrated in Figure 2.4. The power values are taken from the generated lines at the locations of calculation points of the fuel behavior solver. This leaves two problematic points, the inner half of the first volume (closest to the center line of the fuel rod) and the outer half of the last volume (closest to the gas gap). It is not possible to form straight lines at these points without suitable assumptions, as extrapolation has to be made. In this work, it was decided to use a flat assumption for the part closest to the centerline because the power profile is usually very flat for this part in the fuel. In the outer part, the power typically rises sharply near the edge and the shape of the curve is quite often even similar to an exponential function. In this work, however, it was decided to use the calculated value of the preceding line, which was extrapolated to the last half of the volume. In this case, the power at the edge of pellet is slightly underestimated. Power was assumed to be released only into the fuel, i.e. gamma heating or the energy of neutrons scattering in the coolant was not taken into account when determining the location of the released energy.

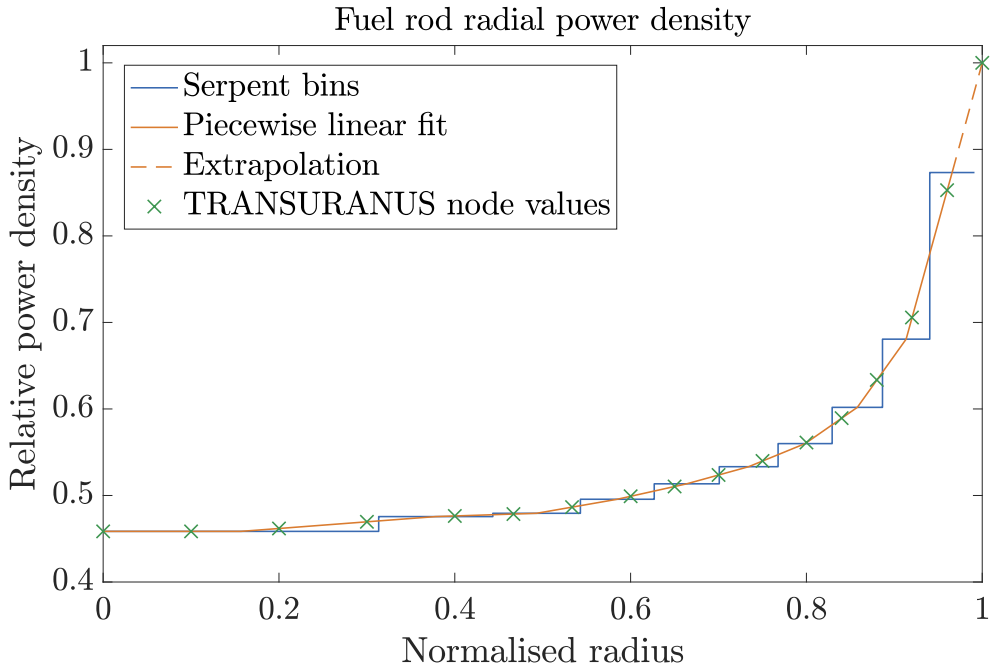

Figure 2.4: Methodology developed for mapping the radial power distribution to TRANSURANUS that smooths out the staircase form resulting from the bin-based power tallies of Serpent.

In coupled calculation, it was essential to select the amount of neutron histories

correctly so that the computing time in Monte Carlo solver remains within appropriate limits. The statistical error of a single solution can be reduced by selecting a larger number of neutron histories, thus reducing iteration times slightly, but on the other hand, increasing the computation time per transport calculation. Anyway, the process is iterative and even if Monte Carlo solution would be ideal, some iterations are needed to reach convergence in coupled computation. Serpent uses relaxation for power during iterations and this approach is based on the stochastic approximation method [24].

In practice, coupling aimed for a few iterations, and if the number seemed to increase to well over 5 iterations, the cut-off condition was thought to be too strict. If the number of iterations varied greatly between different burnup steps, then a large random variation in the results between the iterations might have been impeding the convergence. In such a case, the number of neutron histories should be increased and better statistical accuracy and a further smaller number of iterations could be achieved. Figure 2.5 illustrates the effect of the size of bins and the number of neutron histories on the results of the radial power distribution.

Both power and temperature are used to monitor convergence. On the one hand, the largest single relative change (example given in equation 2.1) is monitored, and on the other hand, the average change of the whole set is monitored in order to follow the total change between iterations over the calculation range. When the changes are small enough, the situation can be considered to have stabilized and additional iterations will no longer have a significant effect on the results. Equation 2.2 shows calculation of l2norm values used to monitor changes in the whole set.

$$\epsilon_i^n = \frac{T_i^n - T_i^{n-1}}{T_i^n}, \tag{2.1}$$

$$\bar{\ell_n^2} = \frac{1}{N}\sqrt{\sum_{i=1}^{N} \left(\epsilon_i^n\right)^2}, \tag{2.2}$$

The basic version of the coupling supported simple burnup calculation with constant extrapolation. This version was used to calculate the NEA-1625 IFPE/GAIN case [25] found in the OECD NEA database. Rods containing burnable poison were known in advance to be problematic for the fuel behavior code reactor physics solver, and in this case such rods have been irradiated, so this case was well suited for demonstration calculation. Research related to coupling of Serpent and TRANSURANUS is presented in Publication III. The main results are presented in section 3.3.

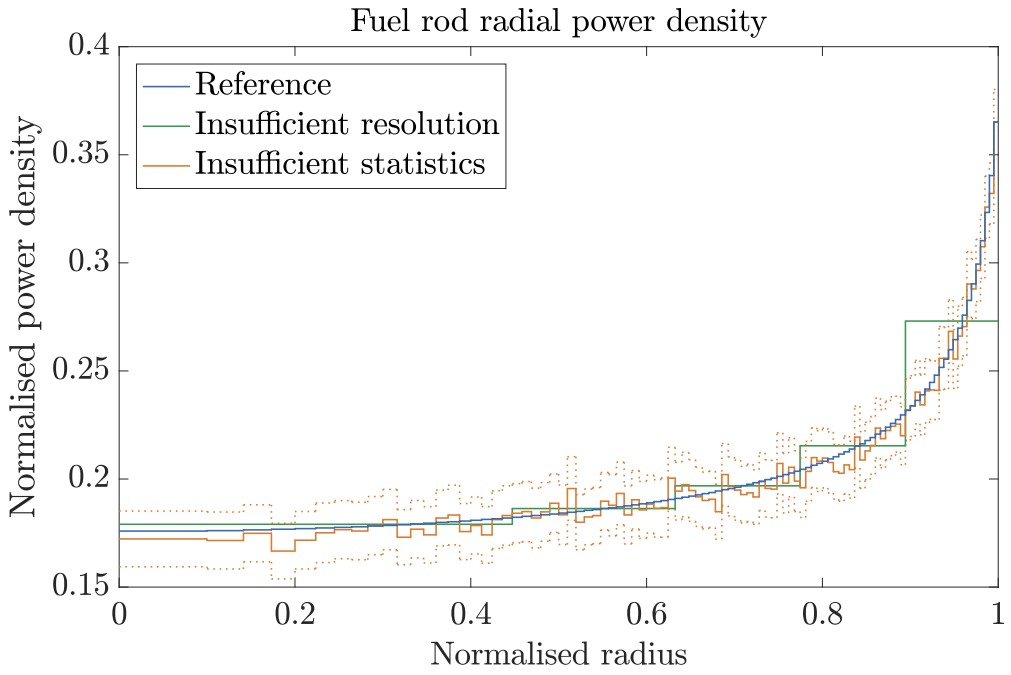

Figure 2.5: Fuel rod radial power density distribution obtained with only 5 bins of equal volume (green) and with 100 bins but too few simulated neutron histories (orange, also showing the 3σ confidence intervals with dotted line) compared to a high resolution (100 bins) reference solution obtained with a massive amount of 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.

2.3.4 Nuclide data transfer in coupling

The Monte Carlo reactor physics code should produce better nuclide concentrations compared to diffusion solver of the fuel behavior code and limited burnup algorithm. It was desired to add the possibility to the coupling code of collecting nuclide concentrations directly from the results calculated by Serpent in addition to the power distribution used in coupling. Serpent includes advanced burnup algorithms and these are described in more detail by Isotalo and Aarnio[26].

The necessary routines for reading nuclide data from the Serpent result files were added to the existing coupling and these results were processed in the coupling code to calculate increments in nuclide concentrations. The fuel code fission product calculation model was modified so that the fission product concentrations it used could be read from the data generated by the coupling code.

In addition, the possibility to use the predictor-corrector type burnup algorithms

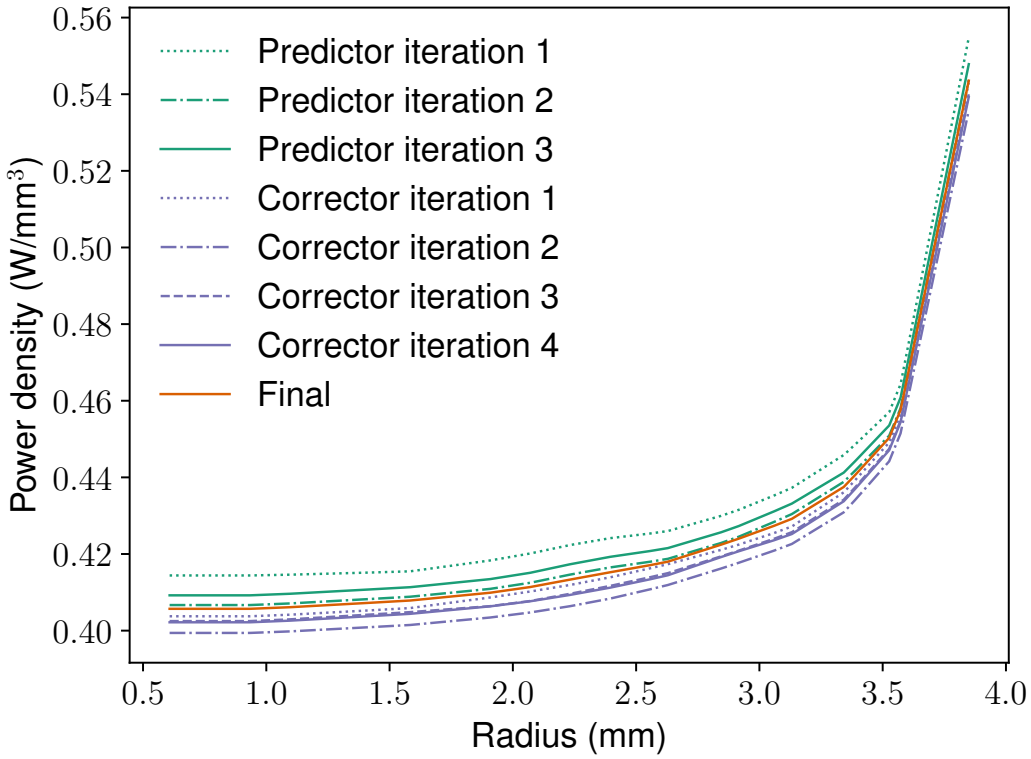

Figure 2.6: Convergence of radial power distribution in the predictor-corrector time integration based burnup calculation. The distributions are for a single axial slice where the total power in iterations is dependent on the convergence of the rod axial power distribution.

was added to the coupling. More specifically predictor-corrector scheme used was linear extrapolation - linear interpolation with substeps[27]. Figure 2.6 shows an example of a convergence process of both phases and its effect on the power distribution. In the end, both can be solved and the average result used in the burnup step is the average of these.

In the case of nuclide concentration calculations, the demonstration calculations were run on the fuel bundle of the Loviisa nuclear power plant. The selected bundle was modeled based on usage history and the bundle contained gadolinium as a burnable poison. Research related to nuclide data transfer is presented in Publication IV. The main results are presented in section 3.4.

CHAPTER 3

Results

3.1 Modeling of randomly packed pebble beds with Monte Carlo

The pebble bed configurations were produced by the discrete element method. The heights of the pebble beds produced and the corresponding experimental core heights are given in table 3.1. There is good agreement with the computed pebble bed heights and measured ones. An example of a pebble bed resulting from a DEM simulation is shown in Figure 2.1 in section 2.2.4.

The formed pebble beds were utilized to create a calculation model for the Serpent Monte Carlo code. The calculation model that has been created is shown in Figures 3.1 and 3.2. Horizontal cut is 60 cm up from bottom of core cavity and axial cut is in YZ direction through origin, which is placed in centerline of reactor.

Serpent calculated the results for multiplication factors for the ASTRA configurations, which are shown in Table 3.2. Sample results are provided with the benchmark documentation and these have been calculated with MCU code. In MCU sample calculation models regular lattice was used for pebble beds and implicit,

Table 3.1: Comparison of the core heights in the experiments and in the calculation model.

Core	Core height in experiment (cm)	Core height in simulation (cm)	Difference (%)
1	179.36 ± 0.53	179.52	0.09
2	214.14 ± 0.53	214.04	0.05
3	291.59 ± 0.48	291.57	0.01
4	320.05 ± 0.41	319.92	0.04
5	421.58 ± 0.19	421.46	0.03

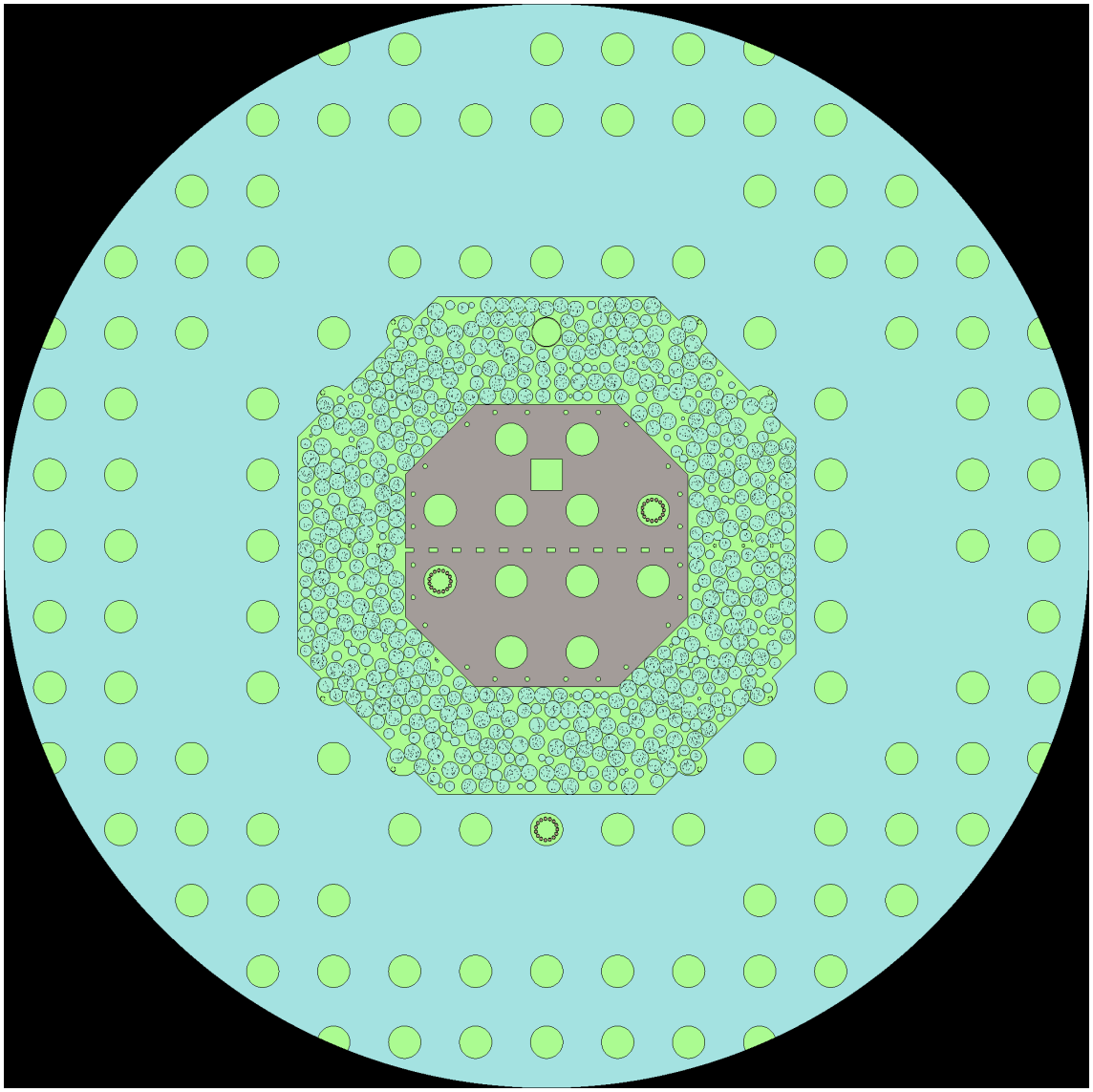

Figure 3.1: Horizontal cross-section of the Serpent model of the ASTRA benchmark case 5. Level of cut is 60 cm up from bottom of the core cavity.

on-the-fly, model for fuel particles.

A computing cluster with Intel Xeon E5-2660 processors was used to calculate the cases. A total of 252 000 000 neutron histories per case was computed, and a maximum of 64 parallel processes were used. These parameters lead to a maximum of 300 CPU − hours used, depending on the case.

The explicit stochastic geometry model used to model the pebble bed structure in Serpent performed as expected. The penalty in computing time of using the explicit stochastic geometry model was 10 % or less compared with the cases

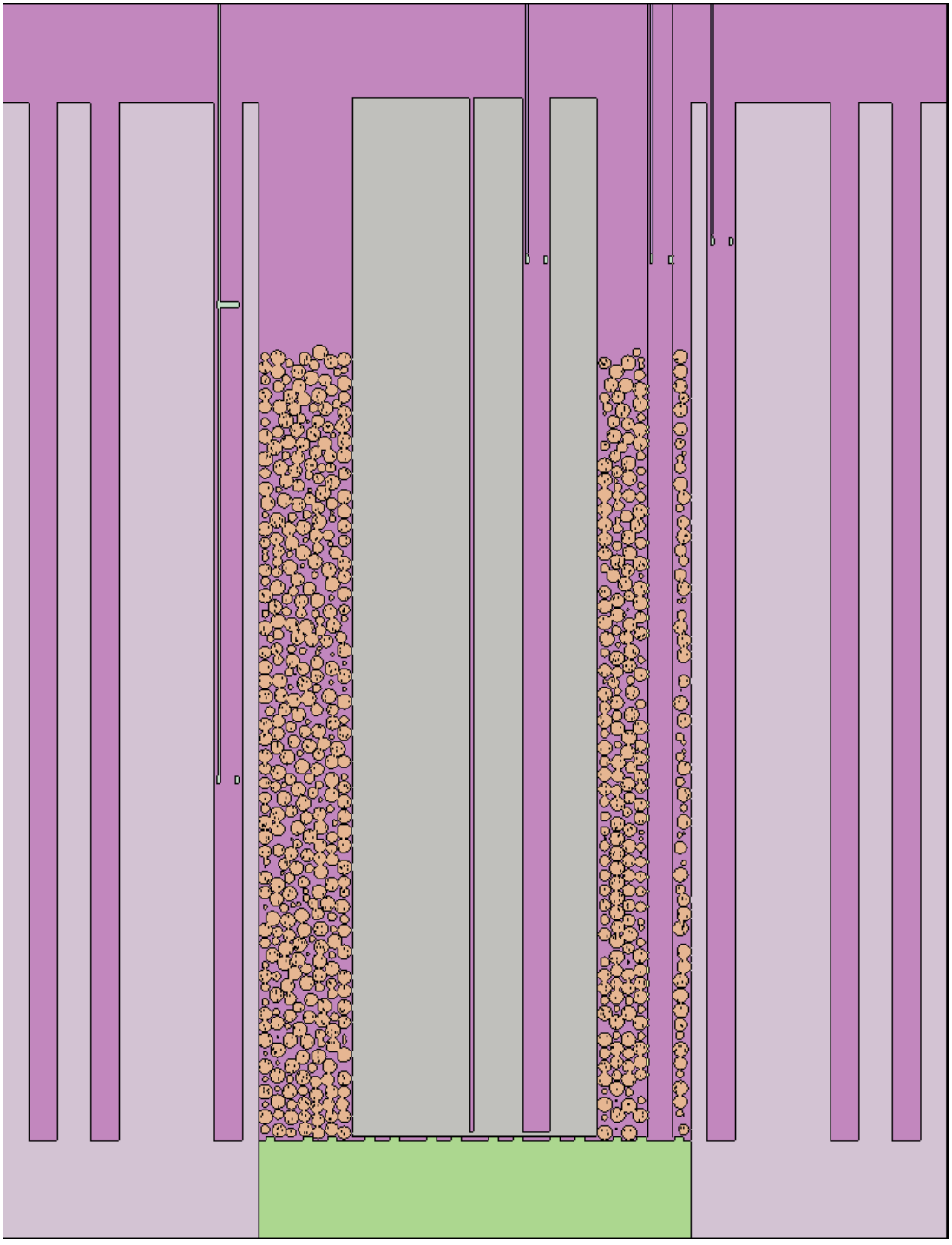

Figure 3.2: Axial cross-section of the Serpent model of the ASTRA benchmark case 4. Cut is in YZ plane and intersecting the axial centerline of the reactor.

Table 3.2: Multiplication factors for different ASTRA configurations.

Core	$k_{eff} \pm 1\sigma$ (experiment)	$k_{eff} \pm 1\sigma$ (sample results) MCU-REA1 DLC/MCUDAT-2.2	$k_{eff} \pm 1\sigma$ (simulation) Serpent 1.1.19 JEFF-3.1.1
1	1.0000 ± 0.0036	0.9912 ± 0.0005	1.00805 ± 0.00008
2	1.0000 ± 0.0036	0.9936 ± 0.0005	1.01038 ± 0.00008
3	1.0000 ± 0.0036	0.9977 ± 0.0005	1.01216 ± 0.00008
4	1.0000 ± 0.0036	0.9989 ± 0.0005	1.01305 ± 0.00008
5	1.0000 ± 0.0036	1.0006 ± 0.0005	1.01403 ± 0.00008

where pebbles and particles are in a regular lattice. This is at least partly related to the fact that neutrons are scattering in graphite and that tracking takes a lot of time. Overall, the penalty caused by the accurate modeling approach seems to be minimal in Monte Carlo reactor physics.

There was bias in the results of the multiplication factors between measured and modeled ones. This was interpreted as being caused by graphite cross-section values. In the calculation models, the impurities in graphite were kept at the same value as in the sample calculation of the benchmark documentation. Depending on the value provided by each cross-section library for the graphite, the amount of impurities should have been fixed to match the measurement results of graphite. First, the graphite impurity content should be calculated by taking graphite cross-sections into account, which means that later in the calculations, the effective cross-sections of graphite match the measured ones. Such measurement data are given for reflector graphite but not for graphite used in fuel. By adjusting reflector graphite to the measurements and making assumptions about the impurity content in fuel graphite, the multiplication factors could be made to be closer to unity.

A more interesting issue in the results was the growing trend of k_{eff} between different benchmark configurations in all the different calculation sets, including the sample calculations provided with the benchmark documentation. We investigated if our modeling approach could explain this trend or part of it, but it seemed to not be related to how the pebble bed was modeled. The trend was very similar between the sample results and our results. On the other hand, this could indicate that something else was needed to explain this trend; here, an explicit modeling approach was in line with other approaches.

The explicit stochastic geometry model was considered to be working, and some other factors in modeling caused the behavior seen in the multiplication factor. Most importantly, the results from this study showed that method seemed to

work correctly. The double heterogeneous structure of the pebble bed seemed to be possible to model without major assumptions; for example, a pebble-wise power distribution could be obtained and used later in coupled calculations.

The structure of the pebble bed was random, as in real reactors, and this did not cause any particular problems with the approach we used. The particle distributions used inside the pebbles were also random. The case example was a zero-power reactor, but despite this, the power distribution was also solvable, which was important from the viewpoint of later research.

Differences in the multiplication factors were observed in the calculations compared with the measured results, but these were because of the differences in the absorption cross-sections of graphite in the material libraries. These values should have been adjusted depending on the library because the direct measurement of graphite impurities is difficult. An equivalent value was determined for the impurities instead, and the absorption cross-section of the graphite of the material library used was taken into account when determining this. The process should be performed separately for each material library used. This was not done, but in the paper, we showed that the differences in multiplication factors were because of the absorption cross-section of graphite.

Otherwise, the results of the calculations followed the sample results given as part of benchmark documentation. It seems that, the growing trend in the multiplication factor according to the height of the pile was because of some unknown reason, other than the modeling of the pebble bed. However, the information available related to the measurement arrangement did not allow for a more detailed examination of the case without a guesswork, and these details were not considered to be of particular importance from the main viewpoint in the research, which was to present a new modeling approach of the pebble bed.

The aim was to model a pebble bed reactor without significant simplifications in the pebble structure, and this was accomplished using a Monte Carlo–type reactor physics code, Serpent, in which the necessary features were implemented by the developers. The aim of the study was to be able to apply a method to pebble bed reactors that takes into account the exact bed structure and that is clearly more advanced than previous calculation codes have been able to provide. This goal was achieved.

3.2 Monte Carlo–based power distribution solution and coupling of thermal hydraulics

In the paper II, a coupled computation that was under development was tested in a case similar to one using an HTR-PM reactor, where a pebble bed was generated with discrete element method. This pebble bed was used in the reactor physics model, and based on the power distribution computed, the temperatures in the

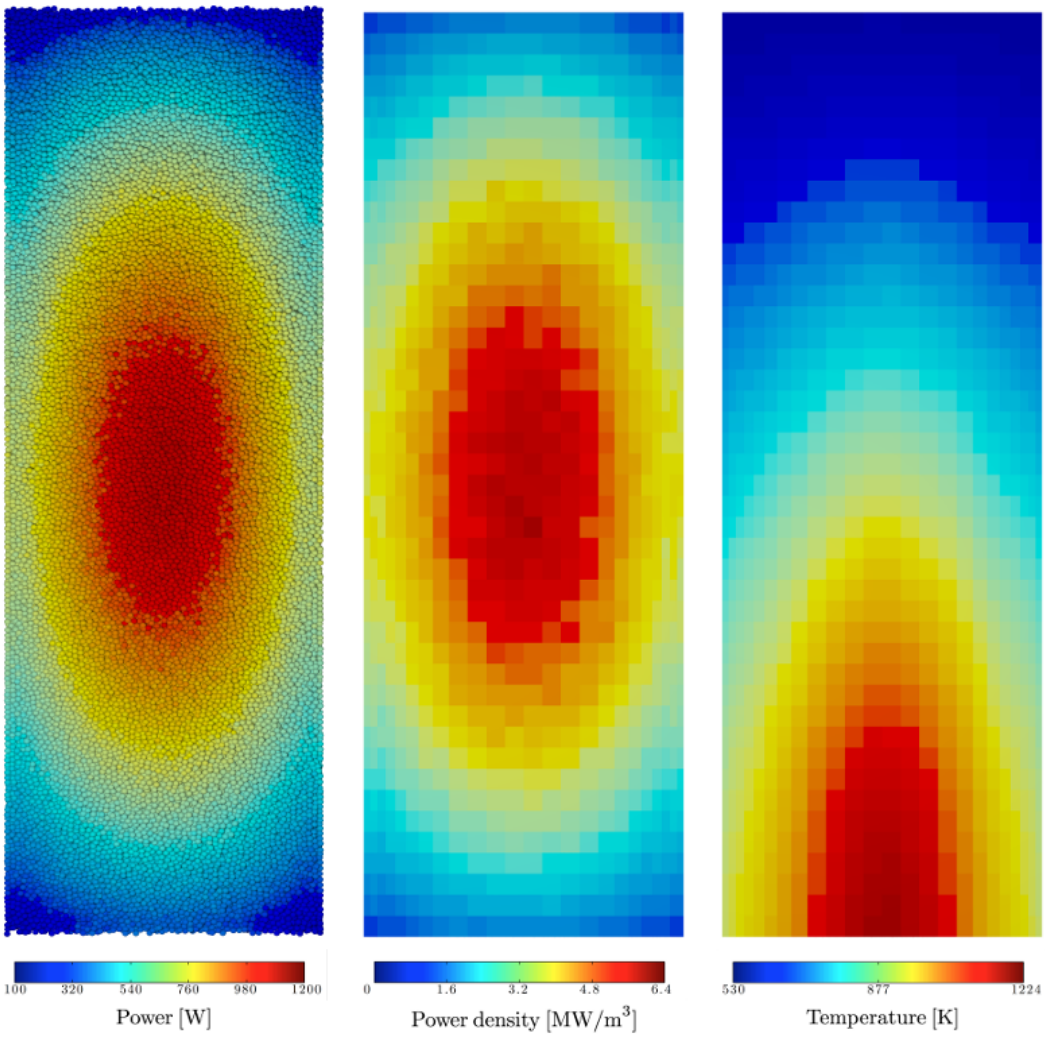

Figure 3.3: Produced thermal power in pebbles as calculated by Serpent (left). Power density mapped into thermal-hydraulic calculation cells (middle). Solid medium surface temperature as calculated by Fluent (right). All plots are taken from the center of the core of the fuel region of the pebble bed.

pebble bed and coolant were calculated using a general purpose computational fluid dynamics (CFD) code. A porosity model was used to model the pebble bed in CFD.

The pebble bed reactor model had about 430 000 fuel pebbles, and the power distribution for this was solved using a method similar to that previously developed for the ASTRA case. Figure 3.3 illustrates the coupled computational process in the form of example results. From the cross-section of the power distribution in the left part of the figure, it can be seen that the power distribution is symmetrical; that is, a uniform temperature distribution in the reactor was obtained and, thus, was an initial iteration. All the fuel in this computation was similar, and the resulting power distribution seemed plausible based on this.

The power per pebble was further subdivided into the calculation cells required by the CFD code using precalculated volume fractions. In the middle of the Figure 3.3, thermal powers are shown in the CFD mesh cells, and the method used to distribute the powers seems functional. Furthermore, based on these power data, the porosity model was used by the CFD code to calculate the surface temperatures of the fuel, which is shown in the same figure on the right. The coolant flow in the primary loop circulates from the top to bottom in the core, and the temperatures are close to correct when taking the power distribution into account.

The most important result was to obtain certainty that a Monte Carlo reactor physics solution could be obtained without a too high computational cost and that the given power distribution was usable in the thermal hydraulic part of calculations. From thermal hydraulics, there was again a clear path to take new temperatures into account in the Monte Carlo reactor physics solution, which completes a single iteration. The coupling code mentioned in this work was developed for these pebble bed reactor calculations, and the underlying functionality was successfully demonstrated in the case of a full-sized pebble bed reactor.

First, this included a one-way coupling between DEM and Monte Carlo reactor physics or thermal hydraulics based on computational fluid dynamics. Second, there is a two-way coupling between reactor physics and thermal hydraulics. A similar approach was used for the pebble bed as previously; that is, the pebble bed was modeled as a double heterogeneous structure that included a randomly packed bed and randomly positioned fuel particles in the pebbles. In addition, the development of an external coupling code for data transfer between the programs started.

The coupled pebble bed demonstration calculation was run with the first version of Serpent, which only had a Doppler preprocessor available to take temperatures into account. Therefore, the amount of memory available to the computers limited the number of different temperature values in the calculations. About 100 different temperature values were used between the extremes to describe tem-

perature distribution in the core. This limitation in the number of total selectable temperatures affects the accuracy obtainable with such an approach, but this was not considered a major problem. There was the possibility to use computers with more memory, and a new version of Serpent was under development. Serpent 2 memory usage is decreased when compared with the previous version thanks to keeping less redundant data in memory. Thus, this limitation of limited temperature zones in modeling was considered solvable if found problematic.

In the coupled calculations of the pebble beds, the calculation cells and locations of the pebbles formed a repetitive structure. It is important for the volume of the pebbles in each cell to be resolved with sufficient accuracy to determine the porosity and distribute power correctly to the cells. If this does not occur, the resulting differences in flow resistance and power will result in repeated differences at the cell-specific temperature in every second cell, here depending on the size ratio between the cells and fuel pebbles. The number of fuel pebbles in each cell is also an important factor, but the size of the cells is usually minimized. This phenomenon has a limited effect on the power output because the geometry on the reactor physics side is accurately described, and the small differences in power of the fuel pebbles at the edges of the cells because of temperature are hardly reflected in the power distribution. The effect could be further reduced by taking into account the temperature differences between the cells, for example, by linear interpolation when determining the surface temperatures of the individual fuel pebbles before the reactor physics calculation. However, caution should be exercised in using such methods because the averaged result can only be used to draw limited conclusions about the exact situation.

In general, the chosen exact modeling approach allowed for the production of an accurate pebble-wise power distribution. The modeling method can be used to produce very accurate results in terms of power distribution, here because of an accurate geometry description and minimal assumptions required. Simplifications of temperature distribution may cause problems, but these are not major obstacles. The alternatives are to use more temperatures, which requires more memory from the computers or a newer version of the Serpent with a multiphysics interface. The multiphysics interface, on the other hand, slows down the computation but uses a similar approach as used in the light water reactor calculations in the present study.

The aim was to find out the possibility of the accurate modeling of pebble bed reactors and determine the usefulness of accurate modeling as part of the coupled calculation. The current study did not find a problem when applying the Monte Carlo method at the level of the entire pebble bed reactor, at least in case of a single calculation point in time.

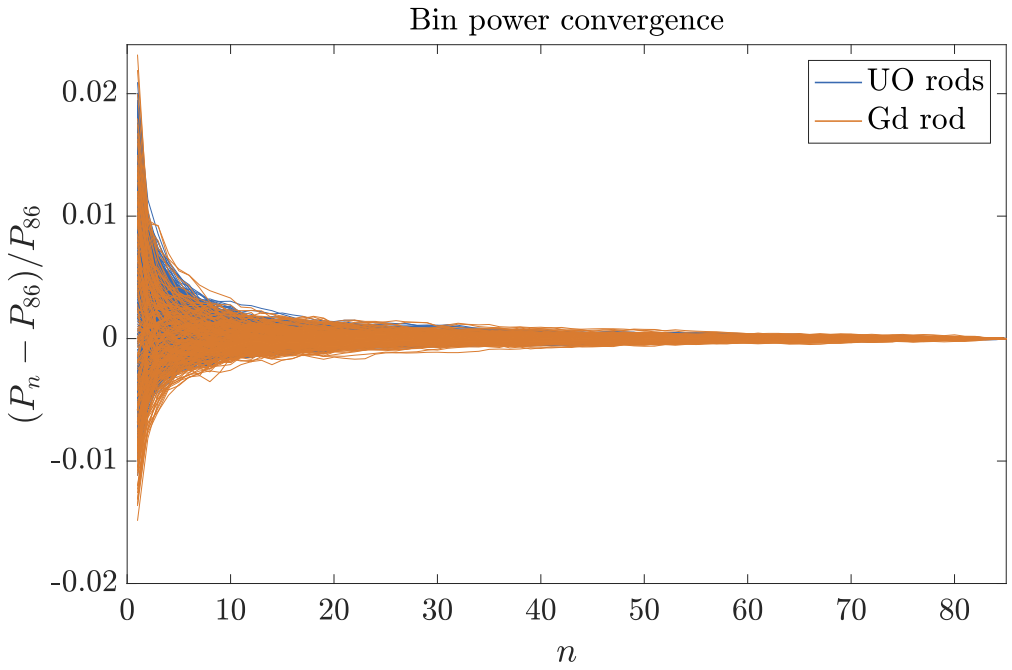

Figure 3.4: Evolution of Serpent bin powers P during iterations. The iteration number is denoted by n. The results are presented relative to the power value of the last calculated iteration step.

3.3 Coupling of Monte Carlo reactor physics with fuel thermo-mechanics

To demonstrate the coupling with light water reactors, the NEA-1625 IFPE / GAIN case available from the OECD NEA databank with four Gd rods irradiated in the Belgian BR3 reactor was calculated. The input data are given in terms of fuel codes and are limited when using Serpent, where the model includes more than just a single rod. One Gd rod was selected for the modeled case, and the calculation model included a 3 x 3 rod grid with eight ordinary UO_2 rods around the center of interest.

Figure 3.4 shows a typical convergence process; it was concluded that the largest changes in the computational results were roughly over after about 10 iteration rounds. The iteration behavior seemed reasonable in general, and the calculation results could be assumed to be good enough by setting the cut-off condition to the value given by the test calculations. This resulted in 7–10 iterations per burnup step.

The computation was run on a single server with 72 computing cores. There were

15 burnup steps, including the first 441 days of irradiation. During this period, burnable poison is burned out of the rod. The computing time was 24.5 days, which corresponds to 9.7 CPU years. This shows the high computing power requirement of the Monte Carlo method. This type of calculation is not intended as a daily computational tool but rather as a way to provide comparative data for the development of computational tools or to solve some special problem.

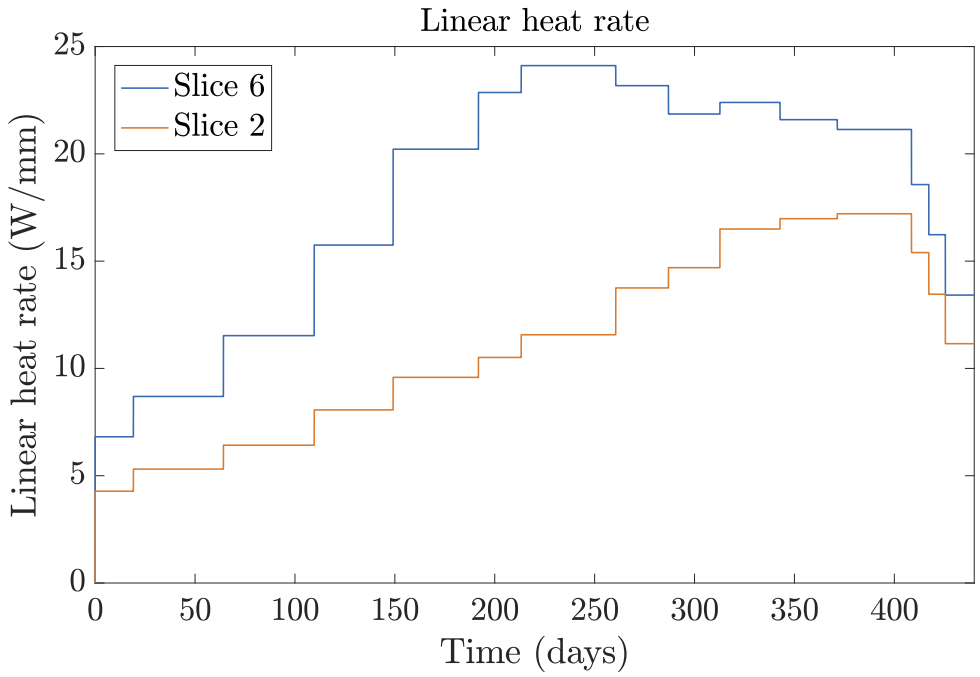

Figure 3.5: Linear heat rates obtained as a result of the coupled calculation for the bottom (Slice 2) and middle (Slice 6) parts of the rod.

Figure 3.5 shows the values of linear power at two axial heights on the rod with different burnups. The results seem reasonable because the central part of the rod has more power (slice 6), and as such, the burnable poison burns out faster than near the edges. The linear power in the middle of the rod starts to decrease after about 250 days, and the burnable poison in the lower part of the rod is burned at a much slower rate. The coupling appears to produce reasonably shaped linear heat rates based on the total rod power, which is given as the initial value.

The results were compared with the corresponding values produced by the fuel code alone. To ensure comparability of the results, the linear power values shown in Figure 3.5 were used in the fuel code and compared with the results produced by the coupling.

Figure 3.6 shows the centerline temperatures in the fuel, which were calculated with the linear powers previously shown. It can be seen from the results that

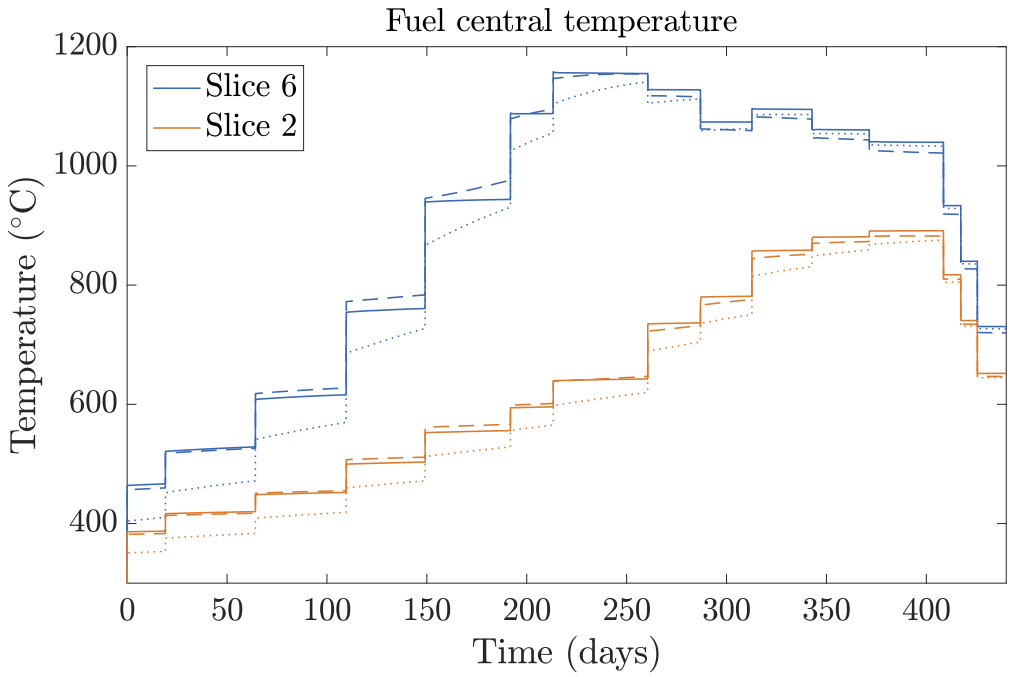

Figure 3.6: Fuel rod's central temperatures during the irradiation period in the bottom (Slice 2) and middle (Slice 6) parts of the rod. Coupled calculation results are plotted with solid. Standalone TRANSURANUS calculation results obtained with the default Gd model (option 1) are shown with dotted lines, and whereas the results with a configuration-specific Gd model (option 102) are shown with dashed lines.

TRANSURANUS produced very different results, here depending on the Gd model used. The results obtained with the coupling were more in line with the results obtained with the configuration-specific Gd model. However, the coupling produced lower centerline temperatures in the inner half of the fuel stack and higher values in the outer half. It should be noted that the linear powers were the same and that the only difference came from the shape of the radial power distribution at different axial positions.

The linear powers were constant over a single burnup step in the calculation. Nevertheless, the centerline temperatures changed during each step because the effective thermal conductivity does not remain constant over a step. The TRANSURANUS results clearly showed a change in temperature within the steps. Time stepping used by TRANSURANUS is much more frequent than the single one used in Serpent. In standalone TRANSURANUS computations, the power is resolved many times during the steps. In the Serpent case, the radial power distribution was found to be constant over a single power step.

In particular, Figure 3.6 shows between 150 and 200 days how the temperature

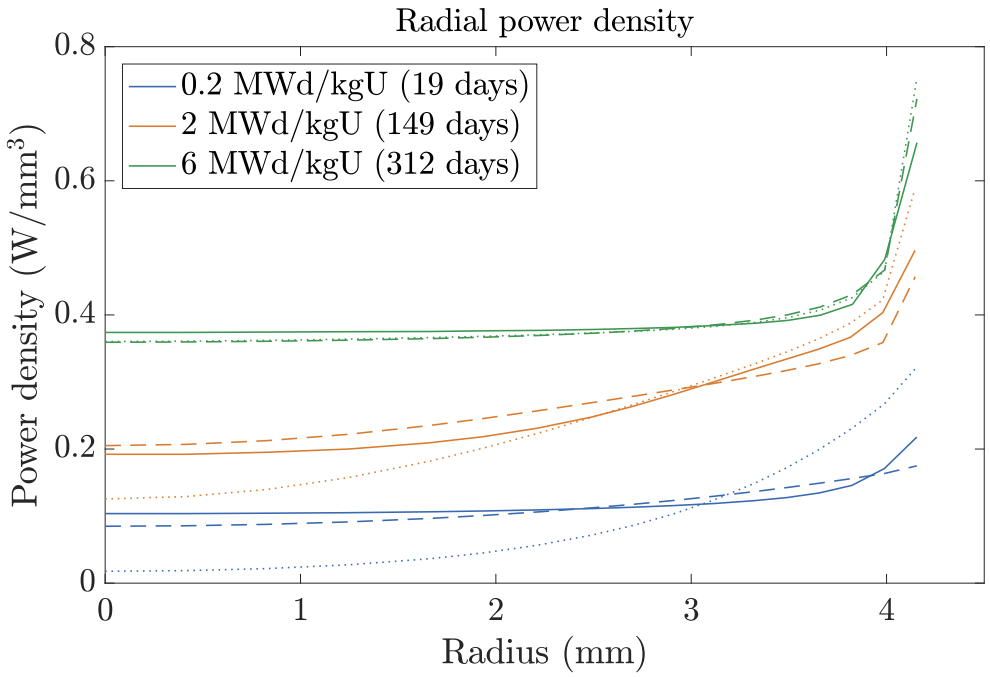

Figure 3.7: Radial power density distribution in the middle part (Slice 6) of the gadolinium-doped fuel rod at different burnups. Coupled calculation results are plotted with solid. Standalone TRANSURANUS calculation results obtained with the default Gd model (option 1) are shown with dotted lines, and whereas the results with a configuration-specific Gd model (option 102) are shown with dashed lines.

increased in the TRANSURANUS during burnup steps. In the coupled calculation, this change was much smaller. The different behavior of the temperatures within the burnup steps may be mainly because of the changes in the effective thermal conductivity or to a different form of radial power distribution within the burnup step. If power is concentrated on the outer edge, the center line temperature should remain lower. In Serpent, the shape of the power distribution did not change, and any changes in temperatures were smaller within each step. Thus, the change in the radial power distribution caused most of this increase. This indicates that the burnup steps in coupling could be shortened to get more up-to-date radial power distributions.

At the centerline, the fuel is the hottest, and the temperature affects various physical reactions or their rates in general. For nuclear fuel, for example, the release of fission gases into the gas space of the rod can be an important quantity; this is increased when the temperature rises. In the inner half, the coupled version seemed to underestimate the centerline temperatures, and in the outer half, the result was overestimated compared with the configuration specific Gd model.

The Gd model of TRANSURANUS may not be perfect, yet it is known that power at the edge of the fuel pellet in the coupling is underestimated.

Figure 3.7 shows the reason for the centerline temperature differences. The radial power distribution is presented at three points in the calculation, and an explanation of the centerline temperatures can be seen in the radial power distribution. If the power is released deeper in the fuel rod, the hotter the centerline temperatures are going to be. The radial power distribution of the coupled computation seems reasonable and was calculated correctly using a Monte Carlo method. The limited resolution near the edge was underestimating power near the surface of the pellet.

Section 3.3 presents the results, where Monte Carlo reactor physics and fuel behavior solver coupling was tested against a case that was intended to be used with traditional fuel behavior solvers. These solvers model typically one pin at a time, which clearly fails in cases where a fuel bundle has different types of pins. In traditional codes, neighboring pins cannot be taken into account without special models. In the case used for demonstration, the history data are provided to the pins of interest, not for the whole geometry, which means that accurate boundary conditions could not be generated for the Monte Carlo model containing neighboring pins. A pin with a burnable absorber was the main interest, and the surrounding normal pins were added to make the calculation model more realistic. These normal pins should improve the flux spectrum in pin containing a burnable absorber. Power normalization was implemented as a given value for the burnable absorber pin, and the calculation model was expected to be a very good presentation of the actual case.

The results show that the coupling seemed to work as intended. The coupled results differed noticeably from the results computed independently by the fuel code with the basic Gd model. This Gd model has been known to have poor accuracy of radial power distribution. The results given by the better Gd model are much closer to the results of the coupled computation. This indicates that coupling has been implemented correctly.

The most significant problem in the calculations was related to the limited number of computational volumes used. If the volumes were not limited, the computation could have taken too much of the limited computational time the when burnup calculations with their necessary iterations were performed. Attempts could be made to improve this result by computing the shape of the power distribution in advance with a reference calculation and using this information to make a better fit, especially near the outer edge of the fuel. It is known that even if the average power of the last computational volume near the pellet edge is correct, the linear fit used to transfer the shape of power density to the fuel behavior code underestimates the power at the edge. This, in turn, leads to a slight

overestimation of the power elsewhere in the pellet because of normalization.

In general, the power solution should be superior to the diffusion solver of the fuel code, and the results obtained should be better than those calculated by a standalone fuel code. The main reason for giving uncertainty is the power distribution shape at the edge, where the limited resolution of the Monte Carlo computational volumes makes it difficult to convey the power distribution shape for the fuel behavior code. At the innermost part of the pellet, the constant value seems to work well enough. By default, Serpent uses equal-volume burnup zones in the rods to produce equally good statistics. Here, a uniform power distribution is assumed, yet in practice, the power in the fuel rods is higher near the outer edge. Reaction rate related weighting of volumes might be part of the solution to this specific problem.

In general, the computational case shows that it is possible to study practical problems with a coupling using the Monte Carlo method. The need for computational power is considerable, so computational times are long. That being said, it is not at all impossible to generate useful results. From the computed results, it can be seen that the coupling using the Monte Carlo method can be used as a high-fidelity result and used further to determine what should be improved in the fuel code power solution for this computational case or the like.

3.4 Nuclide data transfer from Monte Carlo reactor physics to fuel behavior

Support for the transfer of nuclide data between the Monte Carlo solver and fuel behavior code was added to the coupling. At the same time, support for predictor-corrector burnup algorithms was added. A single fuel assembly of the Loviisa power plant (VVER-440) and its operating history were used as an example case. The calculation model contained one bundle with periodic boundary conditions created to form an infinite reactor.

The amount of interesting fission product nuclides was taken directly from the Monte Carlo code. Figure 3.8 shows the difference compared with the results calculated by normal coupling and the fuel code in standalone mode. Standalone calculation of the fuel code gives almost the same result for the formation of fission gases as coupling without nuclide data transfer. In this comparison case, the same power data computed by coupling was used for the rods in TRANSURANUS. The situation changed if Serpent was used as the burnup solver, where both the burnup algorithms and the cross-section data became more accurate than their counterparts in the TRANSURANUS code. It can be seen that the fuel code produced a larger amount of fission gases than the Monte Carlo

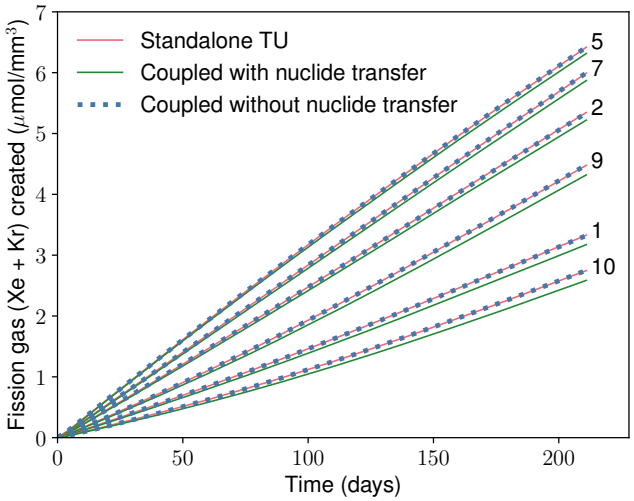

Figure 3.8: Fission gases created during the simulation in selected axial slices. The numbers associated with each set of curves denote the axial slice number from rod bottom (1) to top (10).

solver. However, the differences were small and did not cause clear changes in other important parameters such as fuel rod internal pressure. It must be noted that only the beginning of the fuel irradiation history was computed in the calculations, but the difference would appear to be increasing quite linearly. The result computed by the fuel code appears to be overestimated, at least for these limited burnups, when compared with the result given by the version with nuclide data transfer.

An example of the accumulated amount of xenon in the radial direction is shown in Figure 3.9. It could first be concluded from the figure that the radial and possibly axial power distributions would be different. To exclude this, Figure 3.10 shows the radial power distribution at the corresponding point. The power distributions appear to be very close to each other, and no significant deviation is observed between the coupled calculations.

Thus, the amount of xenon would appear to depend primarily on some factor other than the power distribution, so the difference must be between the burnup algorithms of the programs and the fission yields used. There was no two-way coupling for nuclides in the coupled computation. Such a coupling could improve the computational accuracy by moving nuclides in Serpent burnup zones during computation. The impact of moving nuclides in Serpent may not have a very significant effect, but certainty of this could only be gained by testing. As a main result, the implemented burnup predictor-corrector burnup scheme was working in the coupling and the nuclide data transfer was working

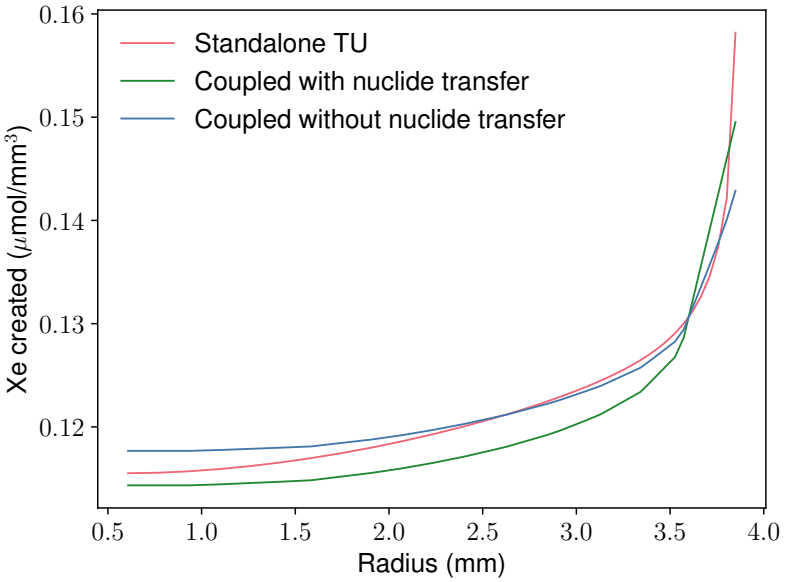

Figure 3.9: Accumulated xenon in axial slice 6 at time 214 days.

to TRANSURANUS. Data transfer was demonstrated by moving increments of those fission products which are used in existing TRANSURANUS models.

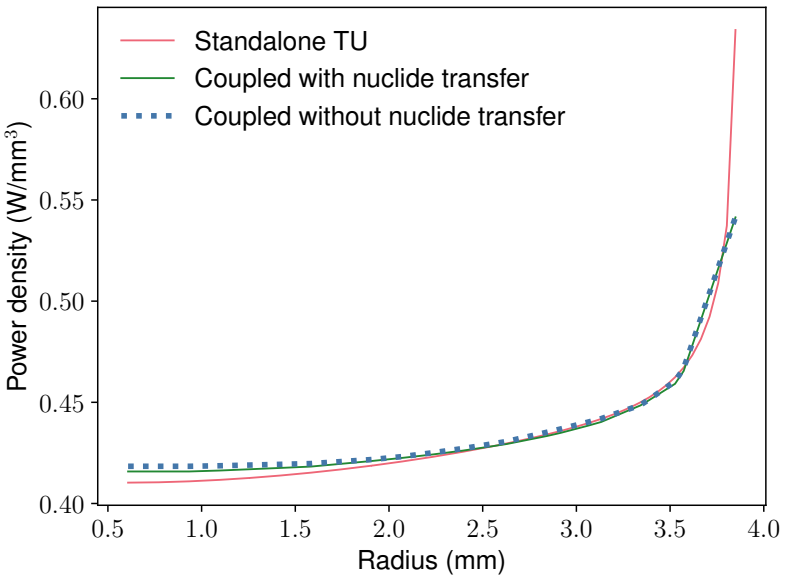

Figure 3.10: Radial power distribution in axial slice 6 at time 214 days.

CHAPTER 4

Discussion

In the current work, the aim has been to improve the accuracy of the calculation methods related to nuclear reactors by using the most accurate known solution method. Cases that are challenging for traditional calculation tools and clearly have room for improvement have been selected as applications. From a research perspective, high-fidelity pebble bed reactor calculations and detailed modeling of light water reactor fuel have been significantly improved.

By using a reactor physics solver of the Monte Carlo type, the uncertainty associated with reactor physics can be mostly eliminated from the calculations. The assumptions made in the calculations are minor, and the sources of errors are largely universal for all reactor physics codes. A clear example of this is the nuclide data that all computational codes use. There are uncertainties associated with the measurements and processing of nuclide data, the effect of which is reflected in the calculation results, regardless of the type of solver.

The calculations presented in the current dissertation have room for improvement in terms of speed. The Monte Carlo reactor physics solution is clearly dominant in the use of computation time, but it can also be very efficiently parallelized. This benefit of concurrency has not been fully exploited because, for example, some time-consuming operations are performed on a serial part of the code. Running the fuel behavior code in the calculations has been serial, too; that is, these computations have used only one processor core. Parallelizing the fuel behavior computation is easy in larger calculation cases because different rods can be solved independently and, as such, simultaneously.

In the case of pebble bed reactors, computational fluid dynamics (CFD) that are used for thermal hydraulics can also be parallelized by dividing the calculation area into parts, here by using domain decomposition. However, the benefit of using parallel computing with a porosity-based solver is quite limited because of the small number of calculation cells. In this case, the overhead related to parallel computing would be comparable with the gained speed. When using the CFD code for a more accurate calculation, where individual pebbles would be present,

parallelization should also be an integral part of the calculation.

By making these fairly simple parallelizations, the computational efficiency can be significantly improved. In recent times, the increase in the computing capacity of computers has largely come from an increased number of computing cores in the processors, and a solver based on Monte Carlo reactor physics can utilize these almost linearly. More detailed analyses of the use of computation time, for example, in the case of Monte Carlo fuel behavior code coupling, have shown that 20 % to 40 % of a computation time is spent on various inefficient input/output (I/O) operations. The actual amounts of data are only low to moderate, and both the solver and coupling code writing operations need to be improved. This share of the calculation time is estimated to be easily reduced to one-tenth of the current one.

On the other hand, the computers used for the calculations were not particularly powerful. For example, there are currently four newer nodes available that have more than twice the computing power of the server used in this paper. If the I/O bottlenecks were corrected, about a third of the original calculation time would be saved. More increased computing power lowers the remaining computing time to less than half. The calculation initially took 24.5 days, and after these changes, it would take 8 days. Monte Carlo computing greatly benefits from parallelism, and an increase in computing power can be expected to continue in the future. This makes the method increasingly suitable for practical problem solving, though it is currently limited as powerful server hardware is still needed. For example, in about 10 to 20 years, the Monte Carlo reactor physics solution may be significantly faster, and the calculations performed for the current dissertation will be successfully performed at powerful workstations.

4.1 Theoretical implications

In pebble bed reactors, the realistic modeling of a reactor core has been developed by utilizing the exact positions of the fuel pebbles. The position information was obtained with a discrete element method (DEM) to be used by the reactor physics solution. In addition, the double heterogeneity problem in pebble bed reactors can also be taken into account for fuel particles, thus avoiding completely making any nonphysical assumptions in the modeling. In the case of the Monte Carlo method, this does not significantly change the calculation time compared with, for example, using homogenized areas or regularly placed fuel pebbles. The approach provides a universal solution to study the behavior of pebble bed reactors, regardless of the level of observation. There is also no need to use time to evaluate errors that may be caused by the nonphysical modeling approaches.

In pebble bed reactors, the coupling of Monte Carlo reactor physics to a thermal-hydraulic solver was also studied; here, it was possible to utilize the obtained power distributions at least in a computation of a single steady state point. The operating cycle length calculation was complicated by the problem of solving the flow of the fuel pebbles, which can be quite computationally intensive with the DEM. Another problem is the large number of burnup zones required in a reactor physics solution, and the depletion process cannot be monitored at the level of a single fuel particle. These separate volumes must be appropriately grouped in one way or another. In the thermal-hydraulic solution, one must stay with the simplest possible model, the porosity model, because the other options are too computationally costly. Other options where the calculation mesh is used to describe the actual pebbles requires the number of mesh cells to increase in such numbers that no maximum imaginable computer capacity of the near future could handle the problem.

For light water reactors, the coupling of reactor physics and fuel behavior code was developed, including a power solution at the fuel rod level. The axial and radial power distributions of the rod are solved in the coupling. The method has been tested from the rod level to the fuel bundle level, and there was no particular restriction on the size of the problem. The main limitation is the availability of computing cores to calculate enough neutron histories. The precalculated coolant temperatures were used as a boundary condition in these calculations. The calculation converged well, and no problems of any kind emerged in the calculations in this respect. Support for fuel codes, other than the TRANSURANUS code used in the current work, can be added to the coupling with reasonable effort.

The Monte Carlo code Serpent has an excellent solver to handle burnup problem; given the accuracy potential of the reactor physics solution, the nuclide compositions to be solved in the burnup calculation should be very accurate. The possibility of nuclide data transfer was added to the coupling, and the possibility of receiving the increments of fission product nuclides was added to the fuel behavior code. This approach can completely replace the fuel code's own limited-accuracy regarding the burnup solver, if desired. Serpent can also track a huge amount of different nuclides, which might be relevant if new models are being added to the fuel behavior code.

4.2 Practical implications

The results can be used for two main purposes: reference results for code development and direct, more accurate analyses with fewer assumptions. In both cases, the benefit is based on the same fact: there is a more accurate method that produces reference results for the applicable problem. These results can be used

to improve simpler and faster but less accurate calculation tools. This is especially true for cases that will be repeated a lot and when a quick solution method is needed. In individual special cases, the problem can be solved directly with this high-fidelity coupling. The end result is a more realistic understanding of the phenomena that limits the use of nuclear fuel and the safety margins based on these limits.

The results will benefit all parties utilizing reactor physics computing, such as reactor physics code developers, plant suppliers, power companies, and nuclear safety regulatory authorities. Increased usage of the methods developed and the additional information they provide will improve the calculation codes at many levels. For example, the fuel behavior code used in the coupling can be further developed so that it behaves more like the coupling when operating in standalone mode. Plant suppliers, power companies, and the authorities can benefit from the results indirectly because of developments in the calculation tools. If necessary, the coupling can also be used directly to solve some special problems, especially if the most reliable solution is needed, for example, to assess the magnitude of specific phenomena in situations where no previous experience exists.

Indirectly, the results will benefit society as a whole because evolving methods will improve the development of concepts currently on the design table, such as small modular reactors, or support the development and use of fuel for existing reactors. These can further enable more efficient and safer use of nuclear fuel. In turn, this can reduce the amount of raw materials needed and amount of high level waste to be disposed in the final repository. All these factors affect the cost of nuclear power and energy production in general.

4.3 Reliability and validity

A reactor physics solution based on the Monte Carlo method makes fewer assumptions than any other solution. It is not necessary to make an energy group division or set restrictions on the directions of neutrons. Possible errors in the results are caused by nuclear data or simplifications in physics modeling; these also affect the results of deterministic computational tools. Taking this into account, the solution given by Monte Carlo reactor physics should be very accurate.

In pebble bed reactor calculations, the reactor core is modeled very accurately to the specifications of a real reactor, and the resulting uncertainty related to the calculation model should be very small. However, these reactors contain a lot of graphite. Material data issues, such as the amount of impurities and uncertainties related to cross-sections, are challenging to calculate. Material-related factors clearly affect the results more than modeling simplifications or improvements.

In the case of pebble bed reactor calculations, the size of the calculation volumes used in the porosity calculation model produces uncertainty. At least 10 fuel pebbles are needed per calculation cell for a porous media assumption to hold. An average temperature value is computed to these volumes, and the effect of small local phenomena on the power output is ignored. Thus, the method is not directly suitable for the detailed studies of small sections. These sections should be modeled separately with a more accurate modeling method to determine the temperatures of the fuel pebbles in the region of interest instead of the average. For example, if the fuel pebbles are very different from each other, then averaging the temperatures in this situation can lead to distortions in the local reaction rates.

Only one steady state point has been considered in pebble bed reactor cases, and conclusions about the generalizability of the method, for example, for the calculation over operating cycle, cannot be made without further reconsideration. The pebble bed reactor can be refueled online, and the pebble bed changes slowly as pebbles pass through the reactor. This kind of pebble flow calculation can be challenging when using the discrete element method because there is no precise information about the need for computational power, but it is nonetheless significant. Solving the pebble flow is a prerequisite for performing the rest of the calculation with the chosen detailed approach and, thus, is a kind of threshold question.

The current work has examined the behavior of the reactor core, and this use is in fact time dependent, in a continuous sense. However, a finite number of time steps have to be used in the calculation codes, which inevitably leads to some inaccuracy. Applying a Monte Carlo reactor physics solution is exceptionally laborious, and the number of time steps should be minimized. In the coupled calculation related to the light water reactors of the present work, where fuel depletion is calculated, the length of the time step is important. During each step, one power distribution is finally obtained after reaching convergence; this should describe the average value over the time step as accurately as possible. For comparison, the deterministic solver of the fuel behavior code can solve the power distribution more often; thus, the modeling of the time dependence can be more accurate. However, the lengths of the burnup steps used are similar to those used in homogenization calculations; the results cannot be completely incorrect, and if they are, the same error will occur in almost all reactor calculations. Considerable work has been done in the development of burnup capabilities in Serpent by developers, and the errors are believed to be small. The feedback effects between coupled codes are delayed when compared with using shorter time steps; when using quick changes, this might be problematic. Xenon concentrations can oscillate in calculations. Here, Xenon equilibrium models are active in Serpent to reduce any unwanted effects when thermal power is being changed. In addition, the shape of the radial power distribution may play a role in the aging of the fuel

pellet structure, and again, the time step should be kept short enough so that the power distribution is not staying at the same constant value for too long.

The number of computational volumes describing the radial power distribution must be kept limited to obtain sufficient statistical accuracy for each region. This ultimately creates uncertainty about the exact shape of the power distribution. In addition, when the power distribution is processed by the coupling code for fuel behavior, the shape of the power distribution is extrapolated linearly according to the last obtained slope on the outer edge of the fuel pellet and with a constant value near the center line. These assumptions are not perfect, but they still work quite well and are simple. After this treatment, the power seems to be slightly underestimated at the outer edge and correspondingly overestimated at the inner part. This results in a slight overestimation of the fuel temperature in most of the fuel rod. The impact is limited, but this needs to be addressed in the future.

Both factors discussed in the last two paragraphs are based on the same issue of limited resolution. One is related to time and the other to place. Compromises have been made for both, as is always the case in modeling. Space resolution is limited, time resolution is limited, and calculations have been made only for the beginning part of the fuel lifetime. Phenomena occurring in the second half of the fuel's service life may require modifications to the coupling. However, nothing special is known that could require major modifications in the coupling code because the methods used are basically very simple. This simplicity is a strength of the Monte Carlo method in terms of accuracy but a weakness regarding the need for computational power.

The results are essentially part of the natural continuum of development work, and the methods are applicable, regardless of reactor type. Applying these methods to different reactor types and situations is a tedious work, but there is no reason why the same methods could not be applied to any reactor type. Different phenomena are known in all reactor types that have not been modeled accurately, which produce computational uncertainties and these must be taken into account in the design and operation of the reactors.

4.4 Recommendations for further research

Easy improvements to coupling calculations of pebble bed reactors include the addition of a suitable multiphysics interface to the Serpent to supply the temperatures of the fuel pebbles. The method should have two steps so that the temperature can also be resolved for the materials of the particles in the fueled zone of the pebbles. This would allow more accurate temperature distributions to be utilized in the calculation, allowing for solving for a more accurate temperature related to

the reactivity feedback coefficients. Currently, Serpent 2 is having more advanced features that allow for taking linear temperature distributions into account. Applying these to pebble bed geometries such as this should be a straightforward task.

The changes in the pebble bed are quite slow, but the reactor can be refueled using online means. In addition, the fuel elements of pebble bed reactors are moving in the reactor core. To model this, a DEM should be used to calculate the flow paths of the pebbles. The next calculation should be run on the reactor physics side with sufficiently short time steps so that the changes in the power distribution caused by the change in the positions of the pebbles can be taken into account with sufficient accuracy. In addition, some material properties may change to such an extent that a two-way coupling between the DEM and rest of the coupling may be necessary to accurately resolve the pebble flow.

There would be a lot to develop on the thermal-hydraulic side of pebble bed reactors, but changing the computation to use a more detailed modeling approach than the porosity model will lead to a significant increase in the computational power requirements. The most useful solution could be to solve the small part of the reactor found to be of interest in the porosity solution, here by utilizing a more precise method and taking the boundary conditions from the porosity solution into consideration. The area of interest could be the hottest calculation cell in the reactor, for example, and this could be modeled in more detail to figure out the stresses experienced by the fuel pebbles in the reactor.

There is also much room for improvement in the coupling of light water reactors and the transfer of the correct shape of the power distribution to the fuel behavior code. The shape of the power distribution could be improved by using a suitable function fit. In addition, the sizes of the calculation areas could be weighted by taking into account the reaction rates, thus improving the resolution in the areas of interest. Reaction rate weighting would make statistical accuracy more constant and does not change the amount of neutron histories being computed.

Another example of improvements is to solve the coolant temperature as part of the coupling. In the current work, the boundary conditions for the coolant were fixed and were a significant constraint from a coupling point of view. At the time of writing the present dissertation, however, support for a subchannel solver has already been added to the coupling, and the mass flow and temperature at the inlet to the core can be used as a boundary condition. This increases the degrees of freedom of the coupling, which means that the state of the reactor core is truly set based on the parameters to be solved in the coupling.

The next improvement in the light water reactor coupling, which is already under construction, is to enable support to a transient-type, time-dependent calculation. In this case, some local time-dependent phenomena can be studied, such as the

movement of the control rods or rapid changes in coolant temperatures. It will then be possible to study problems such as pellet cladding interaction (PCI), for example, when pulling out the control rods in boiling water reactors.

One interesting topic could be to apply coupling in the generation of homogenized group constants and to see if any differences are seen in the group constants itself and on the core-level behavior. Normally, the temperature effects inside of the rod are just omitted. There cannot be major errors in the generation of group constants, but under special circumstances, it might be useful to know the effect of more exact thermal feedbacks.

As a long-term goal, one could consider exploring transient-type safety analyses performed with a coupling utilizing a Monte Carlo-type reactor physics solution. An example could be a control rod ejection type accident. However, this requires considerable amount of computational power and is especially dictated by the solution method used on the thermal-hydraulic side of the coupling.

CHAPTER 5

Conclusions

In the current study, a Monte Carlo-type reactor physics solver was applied to produce power distributions for coupled calculations, here in the case of pebble bed and light water reactors. In pebble bed reactors, the power distribution was produced for each fuel pebble in the reactor, and in light water reactors, calculations were performed at the rod and bundle levels.

For pebble bed reactors, coupled Monte Carlo reactor physics and computational fluid dynamics solution were demonstrated in the case where the discrete element method was used to generate the random structure of the pebble bed. As an example, a single reactor operating point was used, in which a converged solution between powers and temperatures was successfully resolved.

In light water reactor calculations, the starting point was to improve the power solution by taking into account the internal power distribution of the fuel rods. To enable this, an external coupling was created between Monte Carlo reactor physics and fuel behavior codes. The coupling code was created, which handled the functions required for the calculation and data transfer between the codes. Creating this coupling code was a major task. First, the coupling was applied to the modeling of a rod containing burnable poison and later to the fuel bundle of the Loviisa nuclear power plant containing burnable poison pins. In both cases, the power distribution obtained appeared plausible, and the coupling results could be used to improve the accuracy of the fuel behavior solver in standalone mode.

The calculations performed and results show that the reactor physics solution based on the Monte Carlo method can be used as part of a coupled computation. By using fewer assumptions, this method produces more accurate comparison results that can then be used to evaluate the accuracy of faster calculation methods or solve special problems. The calculations are limited by the available computing capacity, but the constant development of computers has already opened up opportunities to apply the Monte Carlo method to practical problems as well.

The advantage of the Monte Carlo-type reactor physics solution is its general applicability; it can be used to model different reactors or fuels without special additional development work. This allows the method to be applied equally well to new applications, hence allowing for a more detailed examination of the development of new types of reactors or fuels. It is still possible to improve resource efficiency and reduce the burden on the environment by increasing the safe and efficient use of nuclear fuel.

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