COMPREHENSIVE FUEL PERFORMANCE MODEL
DEVELOPMENT AND SIMULATION FOR TRISO FUEL

BY

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DISSERTATION

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Abstract

High Temperature Gas Reactor (HTGR), widely recognized as one of the top candidates for the Next Generation Nuclear Power-plant (NGNP) fleet, has received ever-increasing interest due to its superior safety and many other desirable features. TRISO fuel particles are the basic form of the fuel used in both pebble-bed and prismatic reactors. Since they are a key component of the HTGR core design, the success of the reactor depends on the safety and quality of the TRISO particles. During operation, a TRISO particle undergoes complex thermo-mechanical processes. Fission gases accumulate inside the kernel and the buffer layer, and lead to buildup of internal pressure. Uneven thermal conditions lead to asymmetric thermal expansion. The pyrolytic carbon, in both the IPyC and OPyC layers, is known to experience dimensional change (shrinkage or swelling) under fast neutron irradiation. In the mean time, both the IPyC and OPyC layers creep as a function of stress and fast neutron fluence. Macro cracks in the IPyC layer, corrosion in the SiC layer due to chemical attack, and debonding at the interface between IPyC and SiC, have been observed in post-irradiation examinations. All these processes further complicate the stress states in a TRISO particle, and might lead to failure of a single coating layer or the particle as a whole. It is very difficult to duplicate the actual environment that a particle is exposed to in experiments. It is even more difficult to isolate one process from another, thus making it nearly impossible to evaluate the impacts that a particular process has on the fuel particle by conducting experiments. The problem can however at least partially be addressed by modeling and simulation.

Hence, multi-dimensional, multi-physics and comprehensive models are greatly needed to simulate and evaluate the performance of a TRISO particle under normal and accidental conditions. Existing models are inadequate as they are usually one-dimensional
models that over-simplified these processes or do not include all the main physics. The goal of this thesis is to develop a comprehensive, multi-dimensional and multi-physics model to simulate and evaluate TRISO fuel performance. It includes all the main processes taking place in the fuel particle. Three equally important components of this modeling exercise are: 1) 3D heat transfer and temperature distribution analysis; 2) 3D neutronics, heat generation, and fission gas generation and release analysis; 3) 3D stress analysis and failure prediction of the TRISO particle.

The 3D thermal model consists of the solution of the heat conduction equation using the finite difference technique. The temperature calculated using this model is compared to analytical solutions and to the results reported in literature. Good agreements are observed. Thermal models are developed to calculate temperature distribution in a pebble under different power and asymmetric convective boundary conditions caused by, for example, contacts with other pebbles. Three-dimensional temperature distribution in a TRISO particle is also calculated under various conditions such as in the presence of an off-center gas bubble.

Three-dimensional neutronics models are developed using MCNP5/X. Burnup calculations are performed to track the number densities of a few important isotopes and to calculate gas production. The fractional gas release on both intra- and inter-granular level are calculated using the White and Tucker’s model. The gas pressure inside the buffer layer is also quantified.

Finally, 3D axisymmetric stress models are developed using an open-source finite element code, FEAP. Modifications are introduced to FEAP to include PyC shrinkage and creep, etc. The modified code is benchmarked against Miller’s results, and good agreements are observed. A number of variables are studied to evaluate their impacts on stresses and failure probabilities. These variables include creep constant, creep Poisson’s ratio, irradiation temperature, BAF, layer thickness, etc. Some transient thermal conditions such as power surge, and defective cases such as a radial crack in IPyC, debonding and corrosion to SiC, are also studied. Among all, a few variables/conditions have significant impacts on stresses and failure probabilities, namely: shrinkage strain, creep constant, creep Poisson’s ratio, particle size, irradiation temperature, BAF and
cracked IPyC.

Order of magnitude of stresses resulting from temperature changes, pressure buildup due to gas generation, and due to PyC shrinkage/creep show that in the case of TRISO particle (when using specific empirical constants or existing dataset found in literature to calculate shrinkage/creep strains), stresses due to temperature changes and internal gas pressure are orders of magnitude lower than those resulting from shrinkage/creep.

Failure probabilities of both IPyC and SiC are also calculated. The failure probability of IPyC under most conditions borderlines with the design requirement (1E-4) except under low irradiation temperature. The failure probability of SiC under normal conditions is minimal because it is always under compression; except when there is a radial crack in IPyC, in which case the stress in part of SiC becomes tensile and the failure probability is higher than 1E-4, and increases at higher burnup.

The comprehensive fuel performance model developed in this work and implemented in a suite of computer codes simulates the thermo-mechanical behavior of a TRISO fuel particle under irradiation. This work leads to a better understanding of TRISO fuel particle evolution over its lifetime, and provides insights in how to improve the safety and reliability of TRISO fuel. The models developed here can be useful for other purposes related to TRISO fuel or for fuel performance evaluation of other forms of nuclear fuels.
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1 INTRODUCTION*

1.1 Background of TRISO fuel

In an era of high oil prices and fast-growing world energy demand, nuclear energy has received increased interest and is playing an increasingly important role in a country’s energy portfolio. Many countries are moving toward building more nuclear power plants in the near future [1]. Nuclear energy has evolved as a safe, reliable, and economically competitive base-load energy source. It also provides the largest industrial-scale non-emission energy source to combat global warming.

High Temperature Gas Reactor (HTGR), widely recognized as one of the top candidates for the Next Generation Nuclear Power-plant (NGNP) fleet under the U.S. Department of Energy’s Generation IV program [2], has received ever-increasing interest due to its superior safety and many other desirable features. HTGR has high gas outlet temperature which allows for high conversion efficiency, and it is suitable as heat source for hydrogen production and other industrial processes. There are two main HTGR designs: the Modular Pebble-Bed Reactor (MPR) and the Modular Prismatic Helium Reactor (MHR). They both use the tri-structural-isotropic (TRISO) coated particle as fuel, which departs significantly from conventional light water reactor (LWR) fuel designs. This thesis work is focused on pebble bed reactors. Beside energy generation, HTGR is also proposed to transmute transuranic waste by extending fuel’s burnup (so-called Deep Burn), thus reducing geological disposal burden [3].

HTGR is considered safer than conventional light water reactor because of three main aspects:

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* A quick tip to readers: this thesis has an automatic pointer feature. Click on the blue-colored text or number will take you right to the “linked” figure, table, or reference; simultaneously press “Alt” and the left arrow key to return to where you were.
1) It uses helium as coolant instead of water. Helium is chemically inert so it would not corrode fuel or structural materials while water does. Helium remains single phase, while water boils and thus causes thermo-hydraulic instabilities and limits heat transfer.

2) HTGR uses graphite as moderator, and the large amount of graphite, with relatively large heat capacity and high melting point, would act as a huge “heat sink” during accidents such as loss of coolant.

3) The nuclear fuel in HTGR is embedded in tiny TRISO particles with 3 layers of coating, while fuel rods in LWR are surrounded with Zr-alloy cladding. Should there be a crack or a fracture in the coating or cladding, the amount of radioactivity leakage would be much smaller in the HTGR.

One example of HTGR technology is General Atomic’s Gas Turbine-Modular Helium Reactor (GT-MHR) design. This reactor uses direct gas turbine power cycle at high operating temperature, resulting in 50% higher thermal efficiency. Several different forms of fuel were proposed for this reactor such as regular LEU UO$_2$ or MOX, reprocessed LWR spent fuel, weapons surplus Pu or even Thorium, as shown in Fig. 1.1. The high temperature heat output from the reactor can be used for electricity generation, hydrogen production, coal liquefaction and other industrial processes. Another example is China’s HTR-10 project (pebble bed reactor). A test was conducted in 2003 at the HTR-10 to demonstrate the inherent safety of the reactor [4]. During this test, the helium circulator was tripped without scram when the reactor was running at 3MW power. The reactor was able to shut itself down due to the negative temperature reactivity coefficient. The temperature was measured at different core locations and found to be always lower than the 1600°C limit. Based on the HTR-10 experience, a demonstration plant with two 250 MW$_{th}$ HTR reactors (HTR-PM) are being planned to be built, and this plant is projected to commission in 2014 [5, 6].

The TRISO fuel particle is a key component of the overall reactor design and hence its performance is critical to the safety and reliability of the whole reactor. Fig. 1.2(a) shows the structure of a TRISO particle. A TRISO particle has a diameter of around
Fig. 1.1: Several possible forms of fuel to be burned in TRISO-fueled reactors for different applications [7].

0.92 \text{ mm}, with a kernel in the center which is encapsulated by 4 concentric layers. The fissile material resides in the kernel (about 0.5 \text{ mm} in diameter), which is surrounded by a porous carbon layer (Buffer layer), an inner pyrolytic carbon (IPyC) layer, a silicon carbide(SiC) containment layer, and finally an outer pyrolytic carbon (OPyC) layer [8]. The outer layers are designed to act as barriers to contain fission products and as buffers to mitigate impacts caused by fission gas pressure or thermal stress, etc. A tiny TRISO particle is like a micro reactor system that has its own heat generation part and pressure and biological containment. It is crucial that the three coating layers, especially the SiC layer (the strongest one), maintain their integrity during the fuel life, under normal or accidental scenarios. Because once there is a crack through the coating layers, the radioactive isotopes produced in the kernel can easily migrate out of the TRISO particle, travel through the graphite moderator, reach the helium coolant, and then circulate with the coolant over the entire reactor system.
Fig. 1.2: (a) Cut-away schematic view of a TRISO fuel particle [7]; (b) Gas bubbles observed inside high burnup TRISO particle [7].

1.2 The TRISO fuel

During operation, nuclear reactions take place inside the kernel, and fission products are accumulated. Some of them, such as Xe, Kr, He, etc., are in gaseous state. Part of these gases migrate out of the kernel and stay in the porous buffer layer, where the gas pressure keeps building up over time. Fig. 1.2(b) shows the gas bubbles observed inside a TRISO particle with high burnup (747 GWd/tU), and it also shows partial debonding between IPyC and SiC layer [7]. The pressure vessel failure mode has been considered as the main failure mode for TRISO particles by most previous researchers [9–12]. However, significantly greater failure percentage was found in the NP-MHTGR and other coated fuel designed in US than predicted by models that just considered pressure vessel failure [13]. In addition to radial cracks in both PyC layers, partial debonding between the IPyC and the SiC were also found in post-irradiation examination (PIE) [13]. Fig. 1.3(a) shows a radial crack in IPyC observed in PIE. This kind of crack is typical of those observed in PIE of the NP-MHTGR fuel particles [13]. Fig. 1.3(b) shows multiple all-through cracks observed in a failed TRISO particle with high burnup [7]. None of these phenomena can be explained by pressure vessel model alone. Hence, multi-physics models are needed.

Besides the internal gas pressure buildup, a TRISO particle experiences complex
 thermo-mechanical conditions during operation, such as:

- Thermal stress: The temperature within a particle can vary dramatically due to different power levels or boundary conditions. Asymmetric boundary conditions may be due to the fact that particles are packed randomly in the matrix, with the distance between the neighboring particles varying randomly, as shown in Fig. 1.3(b). This kind of uneven thermal conditions will cause uneven thermal stresses. Different coating layers of the particle have different thermal expansion properties, and thus thermal stresses will arise as a result. Gas bubbles inside the kernel and the buffer layer can impede thermal conduction due to their lower thermal conductivity, and thus cause localized elevated temperature at some parts of the particle. The transient processes, such as reactor start up or shut down, power surge, etc., can cause transient thermal stress conditions and thus induce unexpected damage to the particle coatings.

- Shrinkage/swelling of pyrolytic carbon (both IPyC and OPyC layers): Pyrolytic carbon is known to experience either shrinkage or swelling (usually shrinks first and then swells) due to fast neutron irradiation, and the shrinkage/swelling varies with different temperature, fast neutron fluence, and anisotropy/density of the
Fig. 1.4: (a) A diagram of the two different forces (internal gas pressure and the force caused by PyC shrinkage) acting on coating layers. [7]; (b) Kernel migration observed in some TRISO particles [18].

PyC [14–17]. Since the SiC layer is “sandwiched” by two PyC layers, the shrinkage of the PyC would keep the SiC layer in compression. Fig. 1.4(a) shows a diagram of the two different forces (internal gas pressure and the force caused by PyC shrinkage) acting on coating layers [7]. The PyC shrinkage would not necessarily increase the damage to the coating layers, but it has a major impact on the particle stress state and it cannot be ignored.

- Creep of pyrolytic carbon: Pyrolytic carbon is also subject to creep under fast neutron irradiation. The degree of creep mainly depends on neutron fluence, stress conditions and temperature [19,20]. The neutron fluence increases linearly with irradiation time while the stress state of PyC keeps changing, so creep of PyC does not increase linearly with time. Creep would further complicate the stress analysis. Creep as a function of time must be integrated to calculate the accumulated creep. Compared to PyC, the creep and shrinkage of the SiC layer is minimal, so it can be ignored in modelling.

- Defective conditions of the PyC layers: Cracks and thinning in the inner PyC
layer, and debonding at the interface of IPyC and SiC have been observed in post-irradiation examinations [7,13]. These conditions would dramatically change the stress condition in the whole particle, including in the SiC layer.

- Chemical attack to the SiC layer: Palladium, as a fission product, is known to react with SiC to form mechanically weaker compound, thus reducing the effective thickness of the SiC layer [17, 21].

- Swelling of the kernel and shrinkage of the buffer layer: The accumulation of fission gases and elevated temperature can cause the kernel to swell. The buffer layer shrinks because of neutron irradiation. The mechanical changes in the kernel and the buffer layer pose less threat to the overall particle integrity because the buffer layer, as a porous media, acts as a cushion and mitigates the impacts onto other coating layers. But the migration of kernel, as shown in Fig. 1.4(b), can induce asymmetric thermal condition to the overall particle and thus it requires careful evaluation.

It is very difficult to duplicate the actual environment that the particle is exposed to in experiments. It is even more difficult to isolate one process from another, thus making it nearly impossible to evaluate the impacts that a particular process has on the fuel particle by conducting experiments. Besides, irradiation experiments are expensive.

Thanks to the ever-growing computing power, it is feasible to simulate the nuclear, thermo-mechanical processes that a TRISO particle experiences over life time using computer models. To evaluate how a TRISO particle responds to the complex, asymmetric thermo-mechanical conditions, a comprehensive fuel performance model is needed. This model should be multi-physics and multi-dimensional, and it should include most important processes taking place in the particle. It is also desirable that this model be capable of simulating transient processes. Similar goals were recently proposed in a major US DOE project, the Consortium for Advanced Simulation of Light Water Reactors (CASL), for light water reactor fuel performance modelling and simulation [22].
1.3 Existing fuel performance models

Several studies have been carried out to simulate the processes that a TRISO particle experiences, and then to evaluate the fuel performance. Some of these are:

- FZJ model [9]: one of the earliest fuel performance models, which only calculates the *over-pressure* failure of SiC layer but does not include other layers;

- ATLAS [23]: developed by CEA, is a thermo-mechanical model;

- Stress 3 [10]: a stress model, which uses thin shell approximation. The IPyC and OPyC layers were ignored in this model;

- JAERI model [11]: developed at JAERI, is also largely a stress model using pressure vessel assumption;

- PARFUME [24] and TIMCOAT [25]: developed at INL and at MIT respectively, are two fairly comprehensive fuel performance codes for TRISO fuel. Though more advanced than other codes, accuracy of these two codes is however limited due to the 1D modeling for temperature and stress analysis. They also rely heavily on empirical data such as for heat generation and fission gas production rates. The fission gas release model is also somewhat simplified;

- FRAPCON [26]: developed at PNNL, has been accepted as a comprehensive and well-benchmarked fuel performance code. It was however designed for light water reactor fuel rods. It is not applicable to TRISO fuel because of the very different fuel arrangement and geometry.

The nature of the problems that TRISO fuel faces, as described above, are multi-physical and multi-dimensional. The existing models are not adequate and more comprehensive models are needed.
1.4 Overview and objectives of this dissertation

The goal of this thesis is to develop a comprehensive, 3D, multi-physics modelling package, which includes some of the main processes taking place in the fuel, to evaluate TRISO particle performance. Obviously a single PhD work cannot possibly cover every aspect of this subject. Similar work is usually undertaken by a group of researchers at national laboratories. (The CASL project even involves several institutions.)

Fig. 1.5 shows flow diagram of the comprehensive fuel performance code package proposed in this dissertation work. As shown, Three equally important components of this modeling exercise are: 1) 3D heat transfer and temperature distribution analysis; 2) 3D neutronics, heat generation, and fission gas generation and release analysis; 3) 3D stress analysis and failure prediction of the TRISO particle. In addition, two new components, IPyC creep and shrinkage models, have been developed and added into the open-source finite element code, Finite Element Analysis Program (FEAP) which is developed at the University of California, Berkeley [27]. None of these components is independent from others, and they are all connected in one form or another.

1.5 Dissertation outline

This dissertation has been divided into seven chapters. An outline of it is presented below:

In Chapter 2, thermal analysis of the TRISO fuel is presented. A 3D heat conduction model is developed using the finite difference technique. Thermal models are developed to calculate temperature distribution in a pebble under different power and asymmetric convective boundary conditions caused by, for example, contacts with other pebbles. Three-dimensional temperature distribution in a TRISO particle is also calculated under various conditions such as in the presence of an off-center gas bubble.

In Chapter 3, gas production rate in different nuclear fuels are determined. Three
Neutronic model: power, gas and other isotopes generation, fast neutron fluence etc.

Thermal model: temperature distribution in a pebble and a particle at various conditions.

Gas migration and pressure model: gas, radioactivity diffusion, gas pressure cal.

Gas products

Neutronic model: power, gas and other isotopes generation, fast neutron fluence etc.

Fig. 1.5: Flow diagram of the comprehensive fuel performance code package proposed in this dissertation work (the TRISO particle is sometimes referred to as “the particle”).
different nuclear reactors are simulated using coupled MCNP5 and CINDER’90: a fast reactor (SMFR) burning reprocessed transuranic fuel; a high temperature gas reactor (HTGR) burning 20% UO$_2$; and a regular pressurized water reactor (PWR) burning 3% UO$_2$. The capability to track helium production as ternary fission product is added to CINDER’90. The sensitivity of gas production to different fuel composition, fuel enrichment and neutron spectrum are studied as well. Some of the gas production results may be useful to nuclear safeguard applications.

In Chapter 4, burnup analysis of the TRISO fuel is presented. A 3D body-centered-cubic TRISO particle model, with its graphite surroundings and neighboring particles, is developed using MCNPX 2.6.0. All results pertaining to TRISO fuel performance are presented, such as variation of $k_{eff}$, silver/palladium production, variation of fast neutron fluence, etc.

In Chapter 5, gas release analysis of the TRISO fuel is presented. The fractional gas release on both intra- and inter-granular level are calculated using the White and Tucker’s model. The gas pressure inside the buffer layer is also quantified.

In Chapter 6, stress analysis of the TRISO particle is presented. Three-dimensional axisymmetric stress models are developed using an open-source finite element code, FEAP. Modifications are introduced to FEAP to include PyC shrinkage and creep, etc. A number of variables such as creep constant etc. are studied to evaluate their impacts on stresses and failure probabilities. Some transient thermal conditions and defective cases are also studied. Among all, a few variables/conditions are identified to have significant impacts on stresses and failure probabilities. Failure probabilities of both IPyC and SiC are also quantified.

A summary of work and suggestions for future work are given in Chapter 7.
2 THERMAL ANALYSIS OF TRISO FUEL

2.1 Introduction

Among the top six candidates proposed for next generation nuclear power plant, two reactors are given priorities, and the Very-High Temperature Reactor (VHTR) is one of them [2, 28]. For the VHTR concept, the reactor core can be either a prismatic graphite block type core or a pebble-bed core. For the prismatic design, the cylindrical compacts contain thousands of tiny TRISO particles (with a diameter of \( \sim 900 \, \mu m \)) in graphite. And these compacts are then inserted into channels embedded in the graphite fuel assembly blocks. While for the pebble-bed design, the tennis-sized (with a diameter \( \sim 6 \, cm \)) pebbles contain thousands of TRISO particles embedded in graphite as well. And these pebbles are randomly packed inside the reactor core. The TRISO fuel particle is a common component for both designs, and it departs significantly from conventional light water fuel designs. This thesis work is focused on pebble bed reactors. VHTR operates at much higher temperature and higher burnup than PWRs or BWRs. Three-dimensional heat transfer model is a crucial part of the package to capture the TRISO fuel’s thermo-mechanical changes on micro-scale with high fidelity.

Each TRISO particle experiences complex thermo-mechanical processes. Many of these processes are temperature dependent, and thermal gradient is a driving force for some of them. For example, the degree of creep or shrinkage of pyrocarbon is temperature dependent. The thermal conductivities of the fuel and graphite vary with temperature as well. This temperature dependence prevents an analytical solution for the temperature distribution. Temperature dependence can not be assumed to be symmetric, for instance, due to the random contact points where a pebble touches its neighbors (given pebbles are randomly packed together). The off-center gas bubbles inside
a TRISO particle will also cause asymmetric thermal condition. Hence, the thermal analysis should be multi-dimensional. In this work, two new 3D thermal models are developed using finite difference technique; one for the pebble and the other for the TRISO particle. Since TRISO particles are embedded inside pebbles, the pebble thermal model provides boundary conditions for the particle model. The thermal models are benchmarked and tested in three different designs of pebble-bed reactors.

According to the Gen IV technical roadmap, three steps are necessary to pursue the VHTR technology [29]: pilot reactor, demo reactor and the full VHTR reactor. So in this work, the China HTR-10, South Africa PBMR, and the conceptual 600-MW VHTR design are chosen to represent each of the three stages. They differ from each other not just by size, but also by many thermal-hydraulic characteristics. Details of the three reactors are given in later sections.

Finite difference method is used to solve the heat conduction equation in spherical geometry. TRISO particles are embedded inside graphite matrix in pebble balls, so it is natural to solve heat conduction inside the pebble first. Forced-circulated of helium flows through the spaces between pebbles to remove heat, so convective heat transfer boundary condition applies on the pebble surface. Neutron and photon transport simulation is also needed to provide heat generation rates in a pebble as well as in a TRISO particle.

### 2.2 Description: the pebble and the TRISO particle

Fig. 2.1 shows the fuel structure of pebble-bed reactor [18]. This figure shows, from right to left, fuel kernel, TRISO particle, half pebble ball and a few pebbles, respectively. As depicted in the half section of a pebble, thousands of TRISO particles are packed randomly in the inner part of the pebble and there is a graphite “crust” on the surface (5-mm thick). The reactor core is piled with pebbles. Fig. 2.2(a) shows how pebbles are stacked together [18], and Fig. 2.2(b) shows a diagram of helium flowing through a pebble pile [25].
2.2.1 The pebble model

For the thermal model of the pebble, it is impossible to explicitly model each TRISO particle in a pebble (given the large number of particles a pebble contains). Thus, the inner part of the pebble, a mixture of particles and graphite, is assumed to be blended evenly to form a uniform fuel-moderator mix sphere (the volume fraction of each material is preserved), surrounded by a graphite crust. Fig. 2.3(a) shows a diagram of a pebble with the graphite “crust” and a number of TRISO particles embedded inside [25]; Fig. 2.3(b) shows a cross-section of the pebble model for thermal analysis. The outer surface of the pebble is cooled by forced helium flow and thus convective boundary condition applies at the pebble outer surface. Usually the helium flow varies on a pebble surface from one azimuthal angle to another. At the contact points with neighboring pebbles, the helium flow is completely blocked. So the convective boundary condition on the pebble surface is usually asymmetric. Table 2.1 shows dimensions and densities of the two regions. In this work, the particle packing fraction (the volume fraction of all TRISO particles in a pebble) is set as 0.253, as suggested in Ref. [8]. With this packing fraction, a pebble contains about 40,000 TRISO particles.

<table>
<thead>
<tr>
<th>Region</th>
<th>Material</th>
<th>Outer radius (cm)</th>
<th>Density (g/cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>blend of TRISO and graphite</td>
<td>2.5</td>
<td>2.12</td>
</tr>
<tr>
<td>Crust</td>
<td>graphite</td>
<td>3.0</td>
<td>1.74</td>
</tr>
</tbody>
</table>

Table 2.1: Dimensions and material characteristics of the two regions in the pebble thermal model. The inner part of the pebble was homogenized into a uniform fuel-moderator mix region. Note: given the packing fraction of TRISO is 0.253, each pebble contains ~40,000 TRISO particles.

The thermal conductivity of the inner part of the pebble is difficult to evaluate since it is a mixture of particles and graphite. The conventional volume-average method, i.e., weigh the thermal conductivity of each material with its corresponding volume fraction to determine the thermal conductivity of the homogenized region, would induce significant error because this method does not capture the heterogeneous nature of the inner part. Fortunately, there exists an empirical relationship developed by German re-
searchers, as adopted in the German HTR thermal-hydraulic code THERMIX [30]. It is a function of temperature and fast neutron dose, as shown in Eq. 2.1:

\[
\lambda = 1.2768 \left( -0.3906 \times 10^{-4} T + 0.06892 \right) \left( \frac{-0.3906 \times 10^{-4} T + 0.06892}{DOSIS + 1.931 \times 10^{-4} T + 0.105} + 1.228 \times 10^{-4} T + 0.042 \right),
\]

where \( \lambda \) is thermal conductivity (W/(cm-K)), \( DOSIS \) is fast neutron fluence \((10^{21} \text{n/cm}^2)\) and \( T \) is temperature (°C). Based on this relationship, the thermal conductivity of the fuel-moderator region is calculated at a few selected temperatures \( T \) and fast neutron fluences \( DOSIS \), as shown in Table 2.2. From this table, it can be seen that the thermal conductivity decreases significantly from fresh fuel \( (DOSIS = 0) \) to medium burnup \( (DOSIS = 2.5) \), and then stabilizes at higher burnup. This is because fast neutron irradiation induces cavities and interstitials, and the noble gases produced in fission impedes heat conduction. Temperature has a secondary impact on the thermal.
Fig. 2.2: (a) Pile of pebbles (more likely to be randomly packed in reactor core than organized as shown here) [18]; (b) Helium flows through the space between pebbles [25].

Fig. 2.3: (a) Diagram of a pebble with the graphite “crust” and a number of TRISO particles embedded inside [25]; (b) Cross-section of the pebble model for thermal analysis.
conductivity. As for the thermal conductivity of graphite (the crust layer), a wide range of values can be found in literature. Experimental results reported by CEA [31] are chosen for this study. Fig. 2.4 shows variation of the thermal conductivity (W/(mK)) of graphite as a function of neutron fluence at various irradiation temperature [31]. As shown, below some threshold neutron fluence (∼0.4 × 10^{21} n/cm²), the thermal conductivity decreases with temperature. An opposite trend is observed after the threshold. The thermal conductivity of graphite initially decreases significantly with neutron fluence (or burnup) and then slows down. The fact that there is significant amount of graphite in the fueled region as well, explains why similar behavior is observed in both the fueled region and the graphite crust.

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>λ (W/(cm-K))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DOSIS=0</td>
</tr>
<tr>
<td>400</td>
<td>0.4853</td>
</tr>
<tr>
<td>600</td>
<td>0.4070</td>
</tr>
<tr>
<td>800</td>
<td>0.3613</td>
</tr>
<tr>
<td>1000</td>
<td>0.3356</td>
</tr>
</tbody>
</table>

Table 2.2: Selected values of the thermal conductivity (W/(cm-K)) of the fueled region in the pebble at different temperature and fast neutron fluence, DOSIS (10^{21} n/cm²).

2.2.2 The TRISO particle model

For the thermal model of the TRISO particle, each layer is modelled explicitly. Fig. 2.5 shows cross-section of the TRISO particle model for thermal analysis. Asymmetric boundary temperature on the outer surface, caused by asymmetric distribution of neighboring particles, for example, will induce asymmetric thermal condition for the whole particle. The presence of off-center gas bubbles will also induce uneven thermal conditions. The temperature on the particle outer surface is largely determined by the particle’s location in the pebble. The thermal conductivity of UO₂ mainly depends on burnup and temperature, as shown in Fig. 2.6 [32]. Table 2.3 shows dimensions, densities and thermal conductivities of each layer of TRISO [8,17]. The buffer layer is made
Fig. 2.4: Variation of the thermal conductivity ($W/(m\cdot K)$) of graphite as a function of neutron fluence at various irradiation temperature [31].

of porous carbon to hold fission gases, so the thermal conductivity is only around 1/7th that of the kernel. Note that the thermal conductivity of the kernel is taken as the value for UO$_2$ at 700 K with a burnup of 20 GWd/tU in this table.

<table>
<thead>
<tr>
<th>Region</th>
<th>Material</th>
<th>Thickness ($\mu$m)</th>
<th>Density (g/cc)</th>
<th>$\lambda$ (W/(mK))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kernel</td>
<td>14% UC$<em>{0.5}$O$</em>{1.5}$</td>
<td>250</td>
<td>10.5</td>
<td>3.5</td>
</tr>
<tr>
<td>Buffer</td>
<td>porous carbon</td>
<td>100</td>
<td>1.0</td>
<td>0.5</td>
</tr>
<tr>
<td>IPyC</td>
<td>pyrolytic carbon</td>
<td>35</td>
<td>1.9</td>
<td>4.0</td>
</tr>
<tr>
<td>SiC</td>
<td>silicon carbide</td>
<td>35</td>
<td>3.2</td>
<td>30</td>
</tr>
<tr>
<td>OPyC</td>
<td>pyrolytic carbon</td>
<td>40</td>
<td>1.9</td>
<td>4.0</td>
</tr>
</tbody>
</table>

Table 2.3: Dimensions and material characteristics of each layer of TRISO [8, 17] ($\lambda$: thermal conductivity). Note: the overall diameter of TRISO is 920 $\mu$m and the packing fraction of TRISO particle is 0.253.
Fig. 2.5: Cross-section of the TRISO particle model for thermal analysis.

Fig. 2.6: The UO$_2$ thermal conductivity as a function of temperature and burnup calculated using FRAPCON-3 [32].
2.3 1D and 3D numerical models for thermal analysis of the pebble and the TRISO particle

The purpose of developing 1D models is to benchmark the results of our numerical scheme against analytical results. Besides, the 1D models provide quick tests for 3D models. From the thermal energy conservation law and Fourier’s law, we have:

\[
\frac{\partial}{\partial t} (\rho c T) - \nabla \cdot (\lambda \nabla T) = q''''(r,t),
\]

where \( T \) is temperature, \( \rho \) is material density, \( c \) is specific heat, \( \lambda \) is thermal conductivity, and \( q'''' \) is volumetric heat generation rate.

This equation applies to both pebble and particle models. For the purpose of benchmarking in this part of the work, temporal and spatial dependence of thermal conductivity and heat generation are ignored. For steady state, the time-derivative term (the first term) can be ignored, and the resulting equation can be solved analytically in 1D spherical geometry. For the numerical solution, finite difference method (with central difference scheme) is used to solve the governing equation (Eq. 2.2), as shown below:

\[
\frac{r_i^2}{i+\frac{1}{2}} \frac{T_{i+1} - T_i}{\Delta r} - \frac{r_i^2}{i-\frac{1}{2}} \frac{T_i - T_{i-1}}{\Delta r} = \frac{Q}{r_i^2 \Delta r},
\]

where \( Q \equiv -q''''/\lambda \).

Using this numerical scheme, the temperature distribution is calculated and compared to the analytical results for a simple case. In this case, the boundary temperature is set at 800 K and the volumetric heat source is \( 1.19 \times 10^{10} \) W/m\(^3\). Fig. 2.7 shows the comparison of analytical and numerical results. Very good agreement can be seen, showing that the numerical scheme works well. This step provides us as a stepping stone to move toward 3D numerical simulations.

As discussed earlier, 3D model is required to predict the temperature profile inside a TRISO particle or a pebble given the fact that they are almost always likely to be under asymmetric conditions. An analytical solution for the 3D problem is not possible.
because parameters such as thermal conductivity and heat generation are temperature and space dependent. The governing equation, Eq. 2.2, in 3D spherical geometry can be written as (with the time-derivative term ignored for steady state):

$$-r^2 q'''(r) = \frac{\partial}{\partial r} \left( \lambda r^2 \frac{\partial T(r, \theta, \phi)}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \lambda \sin \theta \frac{\partial T(r, \theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial}{\partial \phi} \left( \lambda \frac{\partial T(r, \theta, \phi)}{\partial \phi} \right).$$

(2.4)

Consider the fuel layer of the pebble as an example. The thermal conductivity, $\lambda$ ($\lambda_f$ in this case), is a function of temperature ($T$) and fast neutron fluence ($DOSIS$) given by Eq. 2.1. At certain fuel burnup stage, fast neutron fluence can be assumed to be constant. Temperature ($T$) is a function of $r$, $\theta$ and $\phi$. So we can assume $\lambda_f = \lambda(r, \theta, \phi)$. Second-order central difference technique is used to discretize the second-order derivative term, resulting in the following equation (for brevity, $T(r_i, \theta_j, \phi_k)$ is
denoted by $T(i, j, k)$, and $\lambda(r_i, \theta_j, \phi_k)$ by $\lambda(i, j, k)$:

$$-r_i^2 q_i = \frac{\lambda_{i+\frac{1}{2}} - \lambda_{i-\frac{1}{2}}}{\Delta r^2} (T_{i+1} - T_i) - \frac{\lambda_{j+\frac{1}{2}} - \lambda_{j-\frac{1}{2}}}{\Delta \theta^2} \sin \theta_j (T_{j+1} - T_j) - \frac{\lambda_{k+\frac{1}{2}} - \lambda_{k-\frac{1}{2}}}{\Delta \phi^2} \sin^2 \theta_j (T_{k+1} - T_k) \left(2.5\right)$$

where

$$r_i = i\Delta r, \Delta r = R/L, \ i = 1, 2, 3, \ldots, L,$$

$$\theta_j = j\Delta \theta, \Delta \theta = \pi/M, \ j = 1, 2, 3, \ldots, M,$$

$$\phi_k = k\Delta \phi, \Delta \phi = 2\pi/N, \ k = 1, 2, 3, \ldots, N,$$

$$T_{i+1} = T(i+1, j, k), \ T_{j+1} = T(i, j+1, k), \ T_{k+1} = T(i, j, k+1),$$

$$\lambda_{i+1} = \lambda(i+1, j, k), \ \lambda_{j+1} = \lambda(i, j+1, k), \ \lambda_{k+1} = \lambda(i, j, k+1).$$

By re-arranging, we have:

$$\left(a_i + b_i + c_j + d_j + e_{j,k} + f_{j,k}\right)T_{i,j,k} = a_i T_{i+1} + b_i T_{i-1} + c_j T_{j+1} + d_j T_{j-1} + e_{j,k} T_{k+1} + f_{j,k} T_{k-1} - g_i \left(2.6\right)$$
where

\[
\begin{align*}
a_i &= \frac{\lambda_i + \frac{1}{2} r_i^2}{\Delta r^2}, \quad b_i = \frac{\lambda_i - \frac{1}{2} r_i^2}{\Delta r^2}, \\
c_j &= \frac{\lambda_j + \frac{1}{2} \sin \theta_j + \frac{1}{2}}{\Delta \theta^2 \sin \theta_j}, \quad d_j = \frac{\lambda_j - \frac{1}{2} \sin \theta_j - \frac{1}{2}}{\Delta \theta^2 \sin \theta_j}, \\
e_{j,k} &= \frac{\lambda_{k+\frac{1}{2}}}{\sin^2 \theta_j \Delta \phi^2}, \quad f_{j,k} = \frac{\lambda_{k-\frac{1}{2}}}{\sin^2 \theta_j \Delta \phi^2}, \\
g_i &= q_i r_i^2.
\end{align*}
\]

The values of \(\lambda(i, j, k)\) can be determined by using the results of \(T(i, j, k)\) from previous iteration.

As a result of the periodicity in azimuthal angle, \(\phi\), we have \(T(i, j, N+1) = T(i, j, 1)\), and \(T(i, j, 0) = T(i, j, N)\). Special care is needed to avoid singularity in cases of \(r \to 0\), and \(\theta \to 0\) or \(\pi\). We denote by \(T_0\) the common value of \(T(0, j, k)\), by \(T_{i,N}\) the common value of \(T(i, 0, k)\), and by \(T_{i,S}\) the common value of \(T(i, M, k)\).

For \(r \to 0\) (where \(\bar{\lambda}\) stands for average value),

\[
T_0 = \frac{1}{M N} \sum_{j=1}^{M} \sum_{k=1}^{N} T(1, j, k) + \frac{q(\Delta r)^2}{4 \bar{\lambda}(1, j, k)}.
\]

Similarly for \(\theta \to 0\) or \(\pi\), we have:

\[
T_{i,N} = \frac{1}{N} \sum_{k=1}^{N} T(i, 1, k) + \frac{q(\Delta \theta)^2(\Delta r)^2}{4 \bar{\lambda}(i, 1, k)};
\]

\[
T_{i,S} = \frac{1}{N} \sum_{k=1}^{N} T(i, M-1, k) + \frac{q(\Delta \theta)^2(\Delta r)^2}{4 \bar{\lambda}(i, M-1, k)}.
\]

For the TRISO model, the temperature on outer surface, \(T(L, j, k)\), is taken from the pebble model. While for the pebble model, the temperature on the outer surface is determined by the convective boundary condition.
2.4 Convective heat transfer coefficient in three different designs of pebble-bed reactors

As discussed above, convective boundary conditions are needed for the pebble model. Helium flows around the surface of the ball, as shown in Fig. 2.2(b). On the pebble surface, Robin boundary condition applies:

\[-\lambda \frac{\partial T}{\partial r} |_{R} = h_s (T(R) - T_{He}),\]

where \(R\) is the pebble radius, \(T(R)\) is pebble surface temperature, \(T_{He}\) is helium temperature, and \(h_s\) is convective heat transfer coefficient. (In this equation, heat equilibrium is assumed on the pebble surface: the term on the left hand side represents the heat flux coming from inside the pebble and the term on the right hand side represents the thermal flux carried away by the helium flow.) The convective heat transfer coefficient, \(h_s\), can be determined by the Nusselt Number (\(Nu\)), \(h_s = \lambda_{He} Nu / D_h\). The next step is to determine the \(Nu\).

Based on Achenbach correlation, the appropriate relation for Nusselt Number (\(Nu\)) in gas reactors, as suggested by Dobranich [33], is shown below:

\[Nu = Pr^{1/3}[(1.18Re^{0.58})^4 + (0.23Re^{0.75})^4]^{0.25},\]

where \(Pr\) and \(Re\) are Prandtl number and Reynolds number, respectively, defined as: \(Pr \equiv \frac{\mu c}{\lambda}, Re \equiv \frac{\rho v \bar{z} D_h}{\mu}\). To determine \(Re\), the average helium velocity (\(\bar{v}\)), helium density (\(\rho\)) and hydraulic diameter (\(D_h\)) must be quantified. For the helium flow, a few data points (e.g., helium flow velocity at the core inlet and outlet etc.) are taken from literature rather than solving the complex helium flow for the entire reactor. In addition, specific heat (\(c\)) and thermal conductivity (\(\lambda\)) of helium are needed to quantify \(Pr\). As for the dynamic viscosity (\(\mu\)), the Sutherland’s formula is used: \(\mu = u_0 \frac{T_0 + C}{T + C} \left(\frac{T}{T_0}\right)^{3/2}\), where \(T\) is temperature (K) and \(C\) is Sutherland’s constant. Some of these quantities cannot be known until the specific designs of the reactor are known.

Three representative reactors are chosen to test our codes: HTR-10, PBMR and
VHTR-600. These three reactors are identified as the “three steps” toward advanced
gas reactor technology, as outlined in the Gen IV technology roadmap [29]. Table 2.4
shows the specs of the three reactor designs [34, 35].

<table>
<thead>
<tr>
<th>Item</th>
<th>HTR-10</th>
<th>PBMR</th>
<th>VHTR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal power (MWt)</td>
<td>10</td>
<td>268</td>
<td>600</td>
</tr>
<tr>
<td>Inlet temperature (°C)</td>
<td>250</td>
<td>503</td>
<td>600</td>
</tr>
<tr>
<td>Outlet temperature (°C)</td>
<td>700</td>
<td>908</td>
<td>1000</td>
</tr>
<tr>
<td>Coolant flow rate (kg/s)</td>
<td>3.77</td>
<td>126</td>
<td>288</td>
</tr>
<tr>
<td>Primary pressure (MPa)</td>
<td>3.0</td>
<td>7.0</td>
<td>7.12</td>
</tr>
<tr>
<td>Active core radius (m)</td>
<td>0.90</td>
<td>1.75</td>
<td>2.23</td>
</tr>
<tr>
<td>Active core height (m)</td>
<td>1.97</td>
<td>8.40</td>
<td>8.05</td>
</tr>
<tr>
<td>Max pebble power (W)</td>
<td>600</td>
<td>1379</td>
<td>2112</td>
</tr>
<tr>
<td>Mean pebble power (W)</td>
<td>370</td>
<td>612</td>
<td>1057</td>
</tr>
</tbody>
</table>

Table 2.4: Design specs of the three reactors (HTR-10, PBMR and VHTR) [34, 35].

Helium density is calculated using the equation of state of ideal gas, given by:

\[ \rho = \frac{PM}{RT}, \]  

(2.12)

where \( R \) is the gas constant (8.314 J/(K-mol)) and \( M \) is helium mol mass (4 g/mol). The
hydraulic diameter \( (D_h) \) for triangular lattice (the layout of pebble pile in the reactor
core can be assumed as a triangular lattice), is given by: \( D_h = d \left[ \frac{2\sqrt{3}}{\pi} \left( \frac{p}{d} \right)^2 - 1 \right] \) [36].

In this equation, \( p \) is the average distance between two neighboring pebbles (pitch) and \( d \) is the pebble diameter. Pitch can be determined by using pebble packing fraction, \( p_f \).
The pebble packing fraction is 0.61 for HTR-10 [34], and thus the pitch is calculated
to be 7.18 cm, and this value is assumed for the other two reactors as well. The average
helium velocity (\( \bar{v}_z \)) can be calculated from the mass flow rate:

\[ m_s = S_e \bar{v}_z \rho, \]  

(2.13)

where \( m_s \) is mass flow rate (kg/s), and \( S_e \) is effective active core cross-section area
\((m^2)\). \( S_e \) is defined as \( S_e \equiv S \ast po \), where \( po \) is porosity of the core. Since the pebble
packing fraction is assumed to be 0.61 for all three reactors, the porosity, \( po \), is 0.39.
With all the relations listed above, \( h_s \) can finally be calculated. Table 2.5 shows the average helium velocity (\( \bar{v}_z \)) and the heat transfer coefficient (\( h_s \)) at the inlet and the outlet of each reactor. Note that this is average heat transfer coefficient in a core. It will vary around a pebble surface as a function of \( \theta \) and \( \phi \). See subsection 2.6.2.

<table>
<thead>
<tr>
<th>Item</th>
<th>HTR-10</th>
<th>PBMR</th>
<th>VHTR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet ( \bar{v}_z ) (m/s)</td>
<td>1.50</td>
<td>7.74</td>
<td>12.05</td>
</tr>
<tr>
<td>Outlet ( \bar{v}_z ) (m/s)</td>
<td>2.80</td>
<td>11.78</td>
<td>17.57</td>
</tr>
<tr>
<td>Inlet ( \bar{h}_s ) (W/(m(^2)K))</td>
<td>982.47</td>
<td>3515.88</td>
<td>4321.41</td>
</tr>
<tr>
<td>Outlet ( \bar{h}_s ) (W/(m(^2)K))</td>
<td>868.18</td>
<td>3244.87</td>
<td>4017.10</td>
</tr>
</tbody>
</table>

Table 2.5: Calculated average helium velocity (\( \bar{v}_z \)) and convective heat transfer coefficient (\( \bar{h}_s \)) at the core inlet and the outlet for each reactor.

### 2.5 Heat generation models for the pebble and the TRISO particle

Two relatively simple models are developed to calculate the heat generation distribution in a pebble and in a TRISO particle. For thermal analysis, azimuthal variation of heat generation rate inside a pebble or a particle is not significant, while radial variation is deemed to be important. The asymmetric 3D effects are primarily due to asymmetric boundary conditions and not so much due to asymmetry in heat generation. Rather than time-consuming whole reactor simulation for heat generation calculation, unit-cell models are adopted and they are developed using MCNPX [37].

The heat generation models for the pebble and the particle are similar to their corresponding thermal models: the pebble model has two regions (the inner part is homogenized), and in the TRISO particle model the kernel and the four coating layers are modelled explicitly. Since both particles and pebbles are packed randomly together, Body-Centered-Cubic representation (BCC) is used to represent one pebble or one particle with its neighbors in an average sense. The average distance between two particles or two pebbles is determined by their corresponding packing fractions. Reflective boundary conditions are used in these two models. Fig. 2.8 shows the heat generation
model of the pebble and it includes a pebble and 1/8th of each of its eight neighbors. The space between pebbles is filled with helium; for the TRISO particle model, the space between particles is filled with graphite.

Criticality calculations are performed using MCNPX, and super-imposed $F_6$ mesh tallies are applied to calculate fission energy and neutron/gamma energy deposition in each mesh cell (concentric mesh cells are set up along the radius), and then the total energy deposition in each mesh cell is normalized to the deposition in the outmost mesh cell. Fig. 2.9 shows normalized radial power density profile inside a TRISO particle and in a pebble. In most part of the fuel region, power density is quite uniform in both cases and it decreases towards the edge of the fuel region. For a pebble, there is enough graphite in the fueled region to slow down neutrons; while for a TRISO, its kernel size is very small compared to neutron mean free path, so self-shielding is not significant in either case. In TRISO, power density is lowest in the buffer layer (250-350 $\mu$m) because of its lowest density. The power density gradient in the TRISO is much higher than that in the pebble because neutron can easily “flash” through the thin outer layers of a TRISO particle without depositing energy in them. The power density increases somewhat in the SiC layer (385-420 $\mu$m) because the denser material in this layer has higher stopping power for gamma radiation and thus cause higher gamma energy deposition.

2.6 Results

2.6.1 Temperature distribution in 1D pebble

1D model can be used to solve for the temperature distribution in a pebble if the boundary condition can be assumed to be uniform. A test case was set up to compare this model with results reported in Ref. [34]. In Ref. [34], Gao & Shi used the full-core analysis package THERMIX developed by KFA-Julich [38], which includes several modules covering gas flow and major core components, while the fuel pebble model is one-dimensional. Table 2.6 shows the comparison of max fuel temperature and max
Fig. 2.8: MCNPX model of a pebble and its neighbors using Body-Centered-Cubic representation (reflective boundary condition applied).

Fig. 2.9: Normalized radial power density profile inside a TRISO particle and a pebble respectively. The TRISO particle and the pebble are both divided into several cells, and power generated in each cell is normalized to the power generated in the corresponding outmost cell in the TRISO particle or the pebble.
fuel surface temperature between this work and that by Gao & Shi. In this case, the max temperature is assumed to take place where the coolant is hottest (818°C) and the pebble power is close to maximum (0.52 kW). The results are quite close given the fact that some details are not specified in this reference.

<table>
<thead>
<tr>
<th>Item</th>
<th>this work</th>
<th>Gao &amp; Shi</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max fuel temp. (°C)</td>
<td>917.7</td>
<td>918.7</td>
</tr>
<tr>
<td>Max fuel surface temp. (°C)</td>
<td>870.7</td>
<td>876.7</td>
</tr>
</tbody>
</table>

Table 2.6: Comparison of max fuel temperature and max fuel surface temperature (°C) between this work and that by Gao & Shi [34]. In this case, the max temperature is assumed to take place where the coolant is hottest (818°C) and the pebble power is close to maximum (0.52 kW).

Fig. 2.10 shows the temperature distribution along the radial distance from pebble center for four different cases. For this 1D simulation, symmetric boundary condition is assumed, i.e., the helium is assumed to flow uniformly all around the pebble surface and thus the convective heat transfer coefficient can be assumed to be constant all over the surface in each case. 1D simulations are performed for four cases: PBMR pebble with max (1379 W) and mean power (612 W), and VHTR pebble with max (2112 W) and mean power (1057 W), as shown in Table 2.4. These pebbles are assumed to be located close to the core outlet where the pebble temperature is likely to be the highest. In general, the temperature gradient is smaller in the crust (r > 2.5 cm) because its thermal conductivity is higher than that in the fueled part. Overall temperature drop (∆T) across the pebble for PBMR at mean and max power are 57.2°C and 134.6°C respectively, and the overall drops are 95.4°C and 190.8°C respectively for VHTR. Maximum temperature is 1240°C and 1060°C under max power for VHTR and PBMR, respectively, and it is expected to increase under asymmetric boundary conditions or accidental scenarios. Given that the current operating fuel temperature limit is 1250°C for normal condition and 1600°C for accidental condition [34, 39], the temperature inside the VHTR pebble is very close to the limit. The temperature in the VHTR pebbles can be decreased by reducing power, pebble packing fraction, increasing helium flow rate, or simply by reducing the outlet temperature, etc. As a matter of fact, the recently modified goal
2.6.2 3D temperature distribution in the pebble

In order to test the 3D capabilities of our codes, two asymmetric boundary conditions are set up: Case 1) a pebble is sitting in a uniform uni-directional helium flow, as shown in Fig. 2.11(a); Case 2) a pebble is sitting on top of 3 other pebbles as shown in Fig. 2.11(b) with He flowing downward. Note that the polar angle ($\theta$) is marked up in both figures. 3D simulation results of only VHTR are presented here for brevity.

With the He flow as in Case 1, the problem can be assumed to be 2-dimensional because it is essentially azimuthally (in $\phi$) symmetric. For the convenience of this
Fig. 2.11: Two asymmetric boundary conditions: (a) Case 1, a pebble is in one-directional helium flow [41]; (b) Case 2, a pebble is sitting on top of 3 other pebbles (illustrated with tennis balls). Note that the polar angle ($\theta$) is marked up in both figures.

The study, the convective heat transfer coefficient, $h_s$, is assumed to decrease continuously with the polar angle ($\theta$), and it decreases linearly from $h_{s0}$ at the left most point ($\theta = 0$) to $0.4h_{s0}$ at the right most point ($\theta = \pi$) on the pebble surface (as shown in Fig. 2.11(a)). (More realistic boundary conditions can be easily used once the flow field around the pebble is solved.) The governing equation (Eq. 2.5) is used on a spherical grid with $(r, \theta, \phi)$ in the radial, polar, and azimuthal directions, respectively. All simulations in this part are performed on a mesh of about 3 million grid nodes ($301 \times 101 \times 101$ points in the $r$, $\theta$ and $\phi$ directions, respectively).

Fig. 2.12 shows radial temperature distribution across a VHTR pebble along two different polar angles ($\theta = 0$ and $\theta = 3\pi/4$) under max and mean power. Results from 1D simulations obtained in previous section are also included for comparison. Temperature along $\theta = 3\pi/4$ is always higher than $\theta = 0$ since $h_s$ decreases continuously from $\theta = 0$ to $\theta = \pi$ (except at grid points very close to the pebble center). Compared to the 1D results, the overall pebble temperature is increased significantly due to the asymmetric boundary condition.

In Case 2, the top pebble has 3 contact points, which are assumed azimuthally symmetric, on its surface (see Fig. 2.11(b)). Since the 3 pebbles below partially block the
helium circulation around the top pebble, lower helium velocities are expected in the area surrounding the “south pole” \((\theta = \pi, \text{the lowest point on the top pebble as shown in Fig. 2.11(b)})\). As illustrated in this figure, the 3 contact points share the same polar angle \((\theta = 0.81\pi, \text{as marked in Fig. 2.11(b)})\) and they are distributed azimuthally symmetric \((\phi = 60, 180, 300^\circ, \text{respectively})\). The 3D code can take different convective heat transfer coefficient \((h_s)\) for every surface grid point, if available. If different \(h_s\) is desired for each grid point on the pebble surface, the complex helium flow around the pebble has to be solved first, or it must be solved as a conjugate heat transfer problem. For the purpose of this study — to study how temperature changes in a pebble under different situations— variation of \(h_s\) with \(\theta\) and \(\phi\) is specified explicitly. Fig. 2.13 shows the geometry and the local coordinate for the convective heat transfer coefficient variation around a contact point \((\theta_0 = 0.81\pi \text{ at contact points})\). Remember that there are 3 contact points on the surface of the pebble, and the variation of \(h_s\) around the other two contact points are similar. Heat transfer coefficient \((h_s)\) around a contact point is given...
Fig. 2.13: Diagram of a contact point (θ = 0.81π) and the local coordinate (r) around it.

by:

\[
h_s = \begin{cases} 
0, & r < 0.5 \text{ cm} \text{ (a small ring around the contact points)} \\
0.5 \times h_{g0}, & 0.5 \text{ cm} < r < 1 \text{ cm} \text{ (a larger ring around the contact points)} \\
0.8 \times h_{g0}, & \text{other } \theta > \theta_0 \text{ area (} \theta = \theta_0 \text{ on contact points)} \\
h_{g0}, & \text{the rest of the pebble surface}
\end{cases}
\]

where \( r \) is the radius of the cross-sectional circle as shown in Fig. 2.13.

Fig. 2.14 shows the temperature variation along the polar angle (θ) on the pebble surface in Case 1 and Case 2, each with mean and max pebble power. In Case 1, it is the azimuthally averaged temperature; while in Case 2, it is the temperature along θ for a fixed φ. For Case 1, it shows a clear trend that the pebble surface temperature rises along θ, since \( h_s \) decreases continuously along θ. The max temperature difference on the surface is \( \sim 40^\circ C \) at max power and \( \sim 20^\circ C \) at mean power, respectively. For Case 2, a significant “hump” in temperature can be seen around the contact point (\( \theta = \theta_0 \) (0.81π)), and the temperature also rises after the contact points (\( \theta > \theta_0 \)) because of the deteriorated cooling conditions in area surrounding the “south pole” (\( \theta = \pi \)).

Fig. 2.15(a) shows temperature variation as a function of radius (r) and azimuthal angle (φ) with the polar angle θ fixed at θ₀ (0.81π). It basically shows the temperature on the cone of \( \theta = \theta_0 \), which goes through the pebble center and all 3 contact points as illustrated in Fig. 2.15(b). Three “humps” can be seen on the right edge of the surface plot, where the contact points reside. The influence of the contact points dies away in regions farther beneath the surface (\( r < 2 \text{ cm} \)) of the pebble. The surface temperature
Fig. 2.14: Temperature variation along the polar angle (θ, from 0 to π) on the pebble surface in Case 1 and Case 2. In Case 1, it is the azimuthally averaged temperature; while in Case 2, it is the temperature variation with θ and the azimuthal angle (φ) is fixed at 60, 180, or 300° (that goes through a contact point).

increases significantly on hot spots, although the pebble center temperature increases only by ~10°C due to this asymmetric boundary condition.

2.6.3 3D temperature distribution in the TRISO particle

A 3D test case was also developed for the TRISO particle: a gas bubble was assumed to exist in the TRISO kernel, and it is centered at ($r = 125 \, \mu m$, $\theta = \pi / 4$, $\phi = \pi / 2$). The bubble radius is assumed to be 1/4th of the kernel radius (250 $\mu m$). Since the gas bubble contains mainly Xe, Kr (and a smaller fraction of He), the thermal conductivity of the gas mixture is relatively low (assumed to be 0.02 W/(m-K)) [36]. There is no fission reaction taking place in the bubble so the heat generation is assumed to be zero. Temperature on the TRISO outer surface is set as 900°C (more accurate boundary condition can be set once its exact location inside the pebble is specified). The volumetric power density in the kernel is 1.39E8 W/m$^3$, and it is equivalent to 2.11 kW/pebble (as the VHTR max power case). Fig. 2.16 shows the temperature variation along the radial
Fig. 2.15: (a) Temperature variation of a pebble as a function of radius \( r \) and azimuthal angle \( \phi \) with the polar angle \( \theta \) fixed at \( \theta_0 \). It basically shows the temperature on the cone of \( \theta = 0.81\pi \) (which goes through the pebble center and all 3 contact points on the surface); (b) Diagram of the layout of the 3 contact points and the cone going through the pebble center and the 3 contact points.
distance from the TRISO center at 3 different polar angles ($\theta = 0$, $\pi/4$, and $3\pi/4$, and $\phi$ is fixed at $0.5\pi$). The temperature drop over the whole TRISO is $\sim 13^\circ$C, and it mainly occurs in the kernel and buffer layer because the kernel has high heat source and the buffer has much lower thermal conductivity. The temperature gradient is significant given the TRISO radius is only 460 $\mu$m. The temperature has a “dip” inside the kernel along the polar angle of $\pi/4$ relative to the other two angles, because $\theta = \pi/4$ runs right through the gas bubble. The effect of zero heat source in the bubble is stronger than that of the low thermal conductivity, thus leading to a lower temperature in the gas bubble. Because gas atoms have the tendency of moving towards lower temperature, this temperature variation can partially explain why gas atoms in the fuel migrate into gas bubbles, which seemingly contradicts Fick’s law (gas atoms diffuse from high concentration to low concentration). Temperature along $\theta = 3\pi/4$, which is farther away from the bubble, is almost unaffected by the bubble. Fig. 2.17 shows the temperature variation of the particle as a function of radius ($r$) and azimuthal angle ($\phi$) (with the polar angle $\theta$ fixed at $\pi/4$). As shown, temperature along $\phi = 0.5\pi$ is lower than that along other azimuthal angles because the gas bubble is centered at $\phi = \pi/2$. The presence of the gas bubble does not only affect the temperature within the bubble but also in the immediate “down stream” region. This is because no heat is generated inside the bubble and hence there is smaller heat flux after it.

2.7 Summary

A TRISO particle experiences complex thermo-mechanical changes during reactor operation at high temperatures and under high burnup conditions. TRISO fuel performance analysis requires evaluation of these changes at the micro scale. Since most of these changes are temperature dependent, the thermal modeling of the TRISO fuel is a crucial part of the integral analysis package. In this chapter, a capability has been developed using finite difference technique to determine 3D temperature distributions. Special care has been taken at certain grid points to avoid singularity. Since TRISO
Fig. 2.16: Temperature variation along the radial distance from the TRISO particle center for 3 different polar angles ($\theta = 0$, $\pi/4$, and $3\pi/4$, $\phi$ is fixed at $0.5\pi$).

Fig. 2.17: Temperature ($^\circ$C) variation in a TRISO particle as a function of radius ($r$) and azimuthal angle ($\phi$) (with the polar angle $\theta$ fixed at $\pi/4$). As shown, temperature along $\phi = 0.5\pi$ is lower than other azimuthal angles since the gas bubble is centered at ($r = 125 \mu\text{m}$, $\theta = \pi/4$, $\phi = 0.5\pi$).
particles are embedded inside pebbles for pebble-bed reactor design, 3D models are also developed for pebbles. Complex boundary conditions with convective heat transfer have been studied and applied on the pebble’s outer surface. Numerical results from this model have been compared with analytical results and also with reported results of HTR-10 from literature, and good agreements were obtained. Monte-Carlo models have been developed and heat generation along radial distance inside a TRISO particle and a pebble have been calculated. 3D thermal simulations have been performed for three reactors (HTR-10, PBMR and VHTR). Maximum temperature is 1240°C and 1060°C under maximum power for VHTR and PBMR respectively, and it is expected to increase under asymmetric boundary conditions or accidental scenarios. So modification of VHTR design is needed to make sure max fuel temperature is below 1250°C. Two asymmetric boundary conditions are added to the pebble model to further test the 3D capabilities of the code. Higher temperature was observed at the center and in affected regions. Results are intuitively correct, though further validations are required. A gas bubble was hypothesized inside the TRISO kernel, and 3D simulation was carried out under this scenario. Lower temperature was seen inside the bubble and in the immediate “down stream” region. In short, this work is a stepping stone for this multi-physics fuel performance analysis effort. Future work should include additional validation of the thermal analysis results and also application of more realistic convective boundary conditions on the pebble surface once the helium (coolant) flow is better known.
3 FISSION GAS PRODUCTION IN NUCLEAR FUELS INCLUDING THE EFFECT OF TERNARY FISSION.

3.1 Introduction

A number of gases are produced when uranium and plutonium fission. The most important ones are helium, krypton, and xenon, which make up about 15% of the total fission products. Xenon and krypton are direct products of fission, while helium is mostly produced from the $\alpha$-decay of fission products or transuranics (TRU). In addition, helium can be produced as a direct fission product in ternary fission. With burnup, these different gas atoms can form bubbles in the fuel, both inside the grains and on the grain boundaries. Gas bubbles can have a number of adverse effects on the thermo-mechanical properties of fuel and cladding. They can cause changes in internal gas pressure, thermal conductivity, temperature gradient, and material stress and strain, thus inducing damage or even failure to fuel and cladding materials over time. Hence, evaluation of fission gas impact is a key component for the fuel safety and reliability analysis. An understanding of the mechanism of gas bubble formation, and the effects on fuel performance requires knowledge of the atomic composition of the gases and their production rates.

In this chapter, we present results of simulations carried out to determine the production of the dominant gases in nuclear fuels for different core configurations using MCNP [42] and CINDER’90 [43]. CINDER’90 is a nuclide inventory code, with 63 neutron energy groups, developed at Los Alamos National Laboratory. The main factors that determine the composition of fission gases for different reactor designs are: (1) the burn time, (2) the composition of the fuel, and (3) the neutron energy spectrum. These factors determine the distribution of fission products and their subsequent transmutation into or from stable gases through neutron capture reactions. We consid-
ered three reactor configurations which differ in both fuel compositions and neutron energy spectrum: a high-temperature gas-cooled reactor (HTGR) with 20% enriched UO$_2$ fuel; a sodium-cooled small modular fast reactor (SMFR, developed at Argonne National Laboratory) designed to burn transuranic fuel reprocessed from spent fuel; and a light water reactor (PWR) with 3% enriched UO$_2$ fuel. PWR is one of main commercial reactor types nowadays, while gas reactor and fast reactor are top candidates for next generation power reactor designs [2]. Although the gas production results from only HTGR are needed for our fuel performance modelling for TRISO fuel, it is important to investigate how gases are produced in different fuel compositions. The gas production rate obtained for different fuels are useful for the fuel performance of other fuels. Besides, it is important to test the capability to track gas production of our code package (MCNP+CINDER’90) with different fuels. To enable direct comparisons, the power density was kept fixed at 95 W/cm$^3$ in each case. (The gas production results obtain from MCNP/CINDER simulation are normalized to “per source neutron”. The power density provides a scaling factor. “95 W/cm$^3$” is low, but gas production results for higher power densities can easily be obtained by using a higher scaling factor.) To evaluate the effects on gas production of neutron energy spectrum, separate from fuel composition, we ran a second set of MCNP/CINDER’90 simulations, in which we took the initial fuel to be 3% enriched UO$_2$ for all three reactor types.

3.2 Reactor simulations

The calculations were carried out by coupling the nuclide inventory code CINDER’90 and Monte Carlo neutron/photon transport code MCNP (version 5). CINDER’90, which tracks 3,400 nuclides, including all known direct fission-products (and their daughters), was used to track the gas production. In the case of helium, it was particularly important to track the $\alpha$-decay chains of all actinides and fission products.

Note: in proposed advanced gas reactor designs, the enrichment varies from 10% to 20%. For example, General Atomic’s GT-MHR uses 19.9% enriched UO$_2$ [8]. One of the goal in this work is to quantify gas production in different fuels. 20% enrichment in UO$_2$ is the upper enrichment limit for gas reactor fuel.
Prior to this work, CINDER’90 did not track helium production from ternary fission. This capability has now been added to the library as part of this thesis work (as described in the following subsection). To simplify the calculations, a unit-cell model of each of the three reactor designs was developed in 3D using MCNP5. For both SMFR and PWR, a single fuel rod with its cladding and surrounding coolant channels were modeled. For HTGR, we modeled a single TRISO particle with its 4 coating layers. Reflective boundary conditions were applied in all cases. For the purpose of the gas production studies, accurate determination of the neutron energy spectrum irradiating the nuclear fuel was important, for which a unit-cell model that includes the essence of a reactor core was adequate. Unit-cell modeling has the advantage of high computational efficiency compared to the expense involved in full-core modeling. Criticality calculations, carried out on a 275-processor cluster, were performed to tally neutron fluxes and fission energy deposition. Four million particle histories were sampled in each Monte Carlo simulation. Normalized neutron fluxes, tallied using MCNP5, were fed to the CINDER’90 code which was used to simulate the fuel irradiations. Appropriate magnitudes of neutron fluxes were chosen in each case to reflect the given reactor power level at each time step. Gas production information was then extracted from the results obtained from CINDER’90. In all cases, the fuel is irradiated at a constant power of 95 W/cm$^3$ for a year, and then is left to cool down for another year.

3.2.1 Ternary fission

In a normal fission process, only two fission products are formed when the fissioning nucleus splits in a time interval of $\sim 10^{-14}$ s. While in a ternary fission, three particles are formed in the fission process during this short time period. Ternary fission is of interest to nuclear industry partly because it is an important source of helium, tritium, and hydrogen production in nuclear reactors [44]. Current version of CINDER’90 does not take into account ternary fission. CINDER’90 has 60 fission yield sets, including almost all the actinides from $^{227}$Th to $^{256}$Fm. Since the yield fraction of each fission product depends on the inducing neutron energy, CINDER’90 treats them in three en-
ergy ranges (thermal, fast and high energy). Spontaneous fission is also included. To take into account ternary fission, in this work, helium yield fraction from each of these fissioning actinides at each incident neutron energy level is collected from a LANL report by Madland et al. [45]. This data was processed into CINDER’90 data format and was then added into the CINDER’90 library. After that, some associated parameters are updated (e.g., the total number of fission products is increased by one to count helium) to reflect this new addition to the data library. So if a fissioning nuclide is subject to ternary fission, the modified CINDER’90 produces an extra fission product based on its yield fraction given in the library. Simulations were carried out with this new capability, and the results of ternary fission were compared with benchmark data in literature [45] and good agreement was observed.

3.2.2 High temperature gas-cooled reactor

For the HTGR reactor, we modeled TRISO coated particles. The TRISO fuel particles, are designed to contain all of the fission products. Different designs of the TRISO particle have been proposed by different researchers [7, 8, 17, 46]. When this work was done, a set of TRISO dimensions were chosen as shown in Table 3.1. The outer diameter of the particles is approximately 800 microns in this case. Later on, when TRISO with bigger kernel was found to be more advantageous [8] (easier to manufacture etc.), and adding carbon in the fuel was shown to help reduce CO production, a new set of TRISO dimensions were adopted for all the other parts of this dissertation work. In the present case, the fuel was UO$_2$ with 20% $^{235}$U enrichment, and it contained 1% carbon, as shown in Table 3.2. The fuel also contained a small fraction of boron as a poison.

The TRISO particles are designed to be embedded (in very large numbers) either in graphite pebbles (of pebble bed reactor design), or in graphite matrix to make cylindrical compacts (of modular helium reactor design). For the purpose of determining the fission gas production, the distinction between these two is not significant. We modelled the graphite moderator by adding an artificial graphite layer encompassing the TRISO particle. The thickness of the graphite moderator was set to 153 microns.
<table>
<thead>
<tr>
<th>Item</th>
<th>Thickness (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel kernel, radius</td>
<td>175</td>
</tr>
<tr>
<td>Porous Buffer</td>
<td>103</td>
</tr>
<tr>
<td>Inner Pyro</td>
<td>50</td>
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<tr>
<td>SiC</td>
<td>35</td>
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<tr>
<td>Outer Pyro</td>
<td>43</td>
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<tr>
<td>Total Diameter</td>
<td>812</td>
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</table>

Table 3.1: Dimension of a TRISO fuel particle.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>atom %</th>
</tr>
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<tbody>
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<td>$^{235}$U</td>
<td>6.8</td>
</tr>
<tr>
<td>$^{238}$U</td>
<td>27.2</td>
</tr>
<tr>
<td>C</td>
<td>9.9</td>
</tr>
<tr>
<td>O</td>
<td>56.1</td>
</tr>
</tbody>
</table>

Table 3.2: Isotopic content of the TRISO fuel.

In order to reflect a packing fraction of 0.39 (ratio of the particle volume to the total volume). The neutron flux contributions from the neighboring TRISO particles was treated using spherical reflective boundary conditions. The multiplication factor, $k_{\text{eff}}$, was found to be about 1.5. The power per TRISO particle was $2.13 \times 10^{-3}$ W and the fission rate was $2.92 \times 10^{12}$ fission/cm$^3$·s. The normalized neutron energy spectrum is shown in Fig. 3.1. It agrees well with the results reported in literature [46]. Since the fuel enrichment is relatively high (20%) in this reactor, thermal neutrons are largely absorbed by fuel, and the neutron energy spectrum contains no thermal neutron peak. It does however have an epithermal tail (except for a “dip” around 7 eV due to the high resonance absorption of $^{235}$U around this energy). Note that all neutron energy spectra shown in this chapter are scaled with their own peak (or in other words, the magnitude of neutron flux at most probable energy is always set to one). Hence, the integral of the spectrum over all energies does not necessarily equal one.
3.2.3 Sodium-cooled fast reactor

The Argonne SMFR design has a metallic fueled core with a 30-year lifetime without refueling, and it is designed to burn transuranic (TRU) fuel reprocessed from reactor spent fuel [47]. The high burnup of long-lived radioactive waste is intended to reduce the geological disposal requirements, and to render the waste less weapons usable. The fuel is a U-TRU-10%Zr mixture and the design involves three different TRU fuel enrichment loading zones in order to optimize fuel transmutation and reduce power peaking. In the present calculations, the inner, middle and outer cores were enriched to 10.30%, 14.93%, and 15.96% respectively [48]. The isotopic composition of the TRU is listed in Table 3.3. We modeled a single fuel rod (TRU enrichment 10.30%, where the fuel rod was 1.75-cm in diameter and 100-cm in length). Sodium bond, zirconium alloy cladding and the corresponding sodium coolant channel were all included in the model. The overall cross-section of the model was hexagonal because the fuel rods are arranged in a triangular pattern inside the fuel assembly. The multiplication factor, $k_{\text{eff}}$ is found to be 1.00619 with standard deviation of 0.00019. The normalized neutron
energy spectrum is shown in Fig. 3.2. In this fast spectrum system most neutron reactions occur in the energy range of 0.05–1.0 MeV. The spectrum agrees well with the reported results [49].

<table>
<thead>
<tr>
<th>Isotope</th>
<th>atom %</th>
</tr>
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<tbody>
<tr>
<td>$^{237}$Np</td>
<td>6.73</td>
</tr>
<tr>
<td>$^{238}$Pu</td>
<td>2.78</td>
</tr>
<tr>
<td>$^{239}$Pu</td>
<td>48.99</td>
</tr>
<tr>
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<tr>
<td>$^{241}$Pu</td>
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<td>5</td>
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<td>$^{241}$Am</td>
<td>4.64</td>
</tr>
<tr>
<td>$^{242m}$Am</td>
<td>0.02</td>
</tr>
<tr>
<td>$^{243}$Am</td>
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</tr>
<tr>
<td>$^{243}$Cm</td>
<td>0.01</td>
</tr>
<tr>
<td>$^{244}$Cm</td>
<td>0.49</td>
</tr>
<tr>
<td>$^{245}$Cm</td>
<td>0.04</td>
</tr>
<tr>
<td>$^{246}$Cm</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 3.3: The TRU isotopic content of the U-TRU-10%Zr fuel.

3.2.4 LEU PWR

Finally, we considered a PWR with LEU fuel enriched to 3% $^{235}$U. Table 3.4 shows the composition of this LEU fuel. Table 3.5 shows the dimension of a fuel rod of this reactor. In this model, we included a single UO$_2$ fuel rod with the volume of 101.8 cm$^3$, with Zr alloy cladding and a light water coolant channel. The multiplication factor, $k_{\text{eff}}$, is found to be 1.36909 with standard deviation of 0.0008. Since the volumetric power was assumed to be 95 W/cm$^3$, the power per fuel rod was $9.671 \times 10^3$ W and the fission rate was $2.93 \times 10^{12}$ fission/cm$^3$s. The normalized neutron spectrum is shown in Fig. 3.3, in which the thermal neutron peak is clearly shown at around 0.1 eV.
Fig. 3.2: The normalized neutron spectrum for the Argonne SMFR reactor. The spectrum is dominated by neutrons in the energy range of 0.05 MeV-1.0 MeV.

Fig. 3.3: The normalized neutron spectrum for the 3% $^{235}$U enriched PWR.
<table>
<thead>
<tr>
<th>Isotope</th>
<th>atom %</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{235}$U</td>
<td>1</td>
</tr>
<tr>
<td>$^{238}$U</td>
<td>32</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>67</td>
</tr>
</tbody>
</table>

Table 3.4: The isotopic content of the LEU fuel.

<table>
<thead>
<tr>
<th>Item</th>
<th>Dimension ($cm$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel pin radius</td>
<td>0.4025</td>
</tr>
<tr>
<td>Cladding outer radius</td>
<td>0.4759</td>
</tr>
<tr>
<td>Fuel rod length</td>
<td>200</td>
</tr>
</tbody>
</table>

Table 3.5: Dimensions of the PWR fuel rod.

### 3.3 Gas production

For each reactor configuration we tracked the production of He, Kr and Xe as a function of burn time. To first order, the atom density of each gas grows linearly with the burn time. The results are summarized in Table 3.6. Details of the production rate of individual isotopes for the different reactor designs can be traced to a combination of the fuel content and the neutron energy spectrum. As shown in the table, in all cases, Xe is the dominant gas because of its large yield as a fission product. For example, $^{136}$Xe is produced 6.3 (7.0)% per thermal fission of $^{235}$U ($^{239}$Pu) compared with 1.96 (0.77)% for $^{86}$Kr. In general, Kr has the second largest yield. The largest production mechanism for helium is from the $\alpha$-decay of TRU. Thus the SMFR fuel (with large TRU content in its initial loading) results in an order of magnitude higher helium production than in the HTGR or PWR configurations. Additionally, although the production of helium by ternary fission scales directly with the fission rate, the relative importance of helium production from ternary fission varies from reactor to reactor. The fraction of helium produced from ternary fission is listed in the row “Ternary f.” of Table 3.6. The highest contribution is above 40% in PWR. Since SMFR has the highest TRU in its fuel, it produces most helium from the $\alpha$-decay of TRU. This explains why it has the lowest fraction of helium contributed from ternary fission, as shown in this table. Since HTGR has a harder neutron spectrum than PWR, it has larger yield of TRU, which results in...
higher percentage of helium production from $\alpha$-decay (or lower ternary fission contribution). Fig. 3.4 shows helium production in representative cell of each reactor. As shown in this figure, SMFR has by far the largest production of helium and it continues to build up after reactor shutdown. Note that to count helium production from ternary fission, simulations have been performed with old and new CINDER'90 library (new library has ternary fission data set while old one does not).

Table 3.7 shows the total mass of uranium and plutonium, and burnup (GWd/tHM) at each burn step. Since both HTGR and PWR use UO$_2$ as fuel, there are similar amount of uranium per unit volume and also small amount of plutonium in both reactors. SMFR contains significant amount of plutonium at initial loading in addition to uranium, thus it has higher total uranium and plutonium content. As shown, the final burnup (BU) is less than 4 GWd/tHM. Gas production results at higher BU can be approximately scaled with burnup. However, more accurate results at higher BU cannot be obtained without intensive calculations, since at higher BU, isotopic composition in the fuel will change significantly, and that requires iterative neutron transport and nuclide inventory calculations. These kind of intensive burnup calculations were performed and are reported in the next chapter for the TRISO fuel only.
Fig. 3.5: Production of krypton with burn time for each reactor design (reactor shut down after 365 days).

Fig. 3.5 shows krypton production in each reactor. The production of krypton (either $^{86}\text{Kr}$ or $^{84}\text{Kr}$) from the fission of $^{239}\text{Pu}$ is less than half that from $^{235}\text{U}$, and the production rate of $^{86}\text{Kr}$ ($^{84}\text{Kr}$) from fast fission of $^{238}\text{U}$ is about 65% (82%) that of $^{235}\text{U}$. Thus, the relatively higher plutonium fission fraction results in significantly less (~50% less) krypton being produced in SMFR than in the other two reactor configurations. We also note that as the concentration of $^{235}\text{U}$ decreases and fission contribution from $^{239}\text{Pu}$ and $^{238}\text{U}$ increases with burnup, thus slowing the krypton production rate with time. After sufficient burn time, the burning of $^{239}\text{Pu}$ in PWR (3% $^{235}\text{U}$ enrichment) is greater than that in HTGR (20% $^{235}\text{U}$ enrichment), which lowers the krypton production rate in the case of the PWR.

Fig. 3.6 shows xenon production in each reactor. Since $^{136}\text{Xe}$ is a major component of xenon gas, its production dictates the trend of xenon production as a whole. The production of $^{136}\text{Xe}$ is particularly sensitive to the shape of the neutron spectrum. Because of the extremely large $^{135}\text{Xe}(n,\gamma)$ capture cross section at thermal neutron energies, significantly more $^{136}\text{Xe}$ is produced in reactors where a large fraction of neutrons are in thermal energy range. As a result, nearly 40% more $^{136}\text{Xe}$ is produced in PWR than in the other two reactor designs.
Finally, with the exception of helium production in SMFR, there is very little additional accumulation of noble gases after reactors shut down. In the case of SMFR (with high TRU content in its fuel), $\alpha$-decay almost doubles the total helium inventories after one year of shutdown.

3.4 3% enriched UO$_2$ fuel in all three reactors

The effects of neutron energy spectrum shape on gas production can be examined in more detail by modeling all three reactor configurations with identical 3% enriched UO$_2$ fuel. In all cases the power density was kept fixed at 95 W/cm$^3$ as before. With the change in fuel, $k_{\text{eff}}$ was found to change from 1.5 to 1.36 for the HTGR, and from 1.006 to 0.58075 for the SMFR. All parameters for the PWR were kept unchanged. The gas production results in this hypothetical 3% UO$_2$ were compared to those obtained in their original fuels. Difference in gas production when the same reactor burns different fuels may also provide key information for nuclear safeguard applications. $^{86}$Kr and $^{136}$Xe are two prominent signatures in this regard, besides they give good indication of total Kr and Xe production as well. So in this section, only $^{86}$Kr and $^{136}$Xe, rather than
total Kr and Xe, are reported.

Lowering the $^{235}$U enrichment in the HTGR TRISO fuel from 20% to 3% had a significant effect on the neutron spectrum, and introduced a large thermal peak, as shown in Fig. 3.7. Because the thermal neutron absorption cross section of $^{235}$U is more than two orders of magnitude larger than that of $^{238}$U, the magnitude of the thermal peak scales inversely with the $^{235}$U enrichment. In other words, thermal neutron peak was depressed by the large $^{235}$U absorption in fuel with high $^{235}$U enrichment. In turn, the rate of the $^{135}$Xe$(n, \gamma)$ reaction and the total production of $^{136}$Xe decreases in fuel with higher $^{235}$U enrichment. Fig. 3.8 shows a comparison of the gas production for 3% versus 20% enriched TRISO fuels, where we see a 33% increase in $^{136}$Xe production in the 3% enriched fuel. For krypton, small decrease is observed in 3% enriched fuel since $^{239}$Pu contributes higher percentage of fission in this fuel, and, as discussed above, $^{239}$Pu produces less krypton than $^{235}$U per fission. However, the production of $^4$He for the lower enriched TRISO fuel is only about half of that from higher enriched fuel. Compared with 20% enriched fuel (Fig. 3.7), 3% enriched fuel has smaller fraction of neutron in the resonance region, which implies less production of $\alpha$-unstable TRU, and, thus, less $^4$He production.

Finally, in the case of the SMFR, the change in the shape of the neutron spectrum is shown in Fig. 3.9, where it can be seen that the spectrum becomes softer. As shown in Fig. 3.10, the production rate of helium changed significantly when the $^{238}$U+10%TRU fuel was replaced with 3% enriched UO$_2$. But the main effect on helium production is the lack of TRU in the initial fuel loading, which translates into less $\alpha$-decay. As a result, the helium production drops by about a factor of three. Also note that the production rate of $^4$He decreases 30 days after reactor shut down since some of the short-lived $\alpha$-emitters decay out. The 3% enriched UO$_2$ fuel is dominantly burning $^{235}$U, while the TRU fuel is dominantly burning $^{239}$Pu and $^{241}$Pu. Fig. 3.10 also shows the comparison of $^{86}$Kr and $^{136}$Xe production in these two different fuels. Production of $^{86}$Kr was doubled in 3% enriched UO$_2$ fuel because $^{235}$U has twice the $^{86}$Kr yield than that of $^{239}$Pu or $^{241}$Pu. For $^{136}$Xe production, a small change was observed, but the neutron energy spectrum did not change significantly and the fission yield of $^{136}$Xe
Fig. 3.7: Comparison of the neutron energy spectrum in HTGR with: 3% (dashed line) vs. 20% (solid line) enriched UO$_2$ fuel.

Fig. 3.8: Comparison of the noble gas production in HTGR: 3% (dashed line) vs. 20% (solid line) enriched UO$_2$ fuel.
is similar in $^{235}\text{U}$ and $^{239}\text{Pu}$.

### 3.5 Summary

Gas production rate is an important input in determining fuel performance. The noble gas production for a number of reactor configurations was examined. In all cases, the gas production scales approximately with burn time, and xenon is by far the dominant gas. With the exception of burning TRU, krypton has the second highest production rate, but is typically an order of magnitude less than xenon. Helium is produced at a rate of roughly $1/50^{th}$ of xenon, except in the case of burning TRU, where ten times more helium is produced, and the helium atom density is about $1/5^{th}$ that of the xenon and three times that of krypton. $^{136}\text{Xe}$ can be produced significantly more in reactors where there is a strong thermal neutron peak because of the large cross section of the $^{135}\text{Xe} (n, \gamma)$ reaction at thermal energies. In the present calculations, a fixed power density of 95 W/cm$^3$ was assumed, and the gas densities listed in Table 3.6 were scaled with this power density. The MCNP-CINDER’90 code package provides an inexpensive means.
of accurate gas production estimates in different reactors with the desired temporal and spatial resolution. The vast datasets included in the CINDER’90 libraries allow one to track the irradiation-induced production and depletion of thousands of isotopes, including the noble gases examined here.

The gas production results reported here provide valuable dataset to evaluate and address the adverse effects on nuclear fuel and cladding due to fission gases accumulation. Difference in gas production, e.g., $^{86}$Kr and $^{136}$Xe, when the same reactor burns different fuels may also provide key information for nuclear safeguard applications.
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<th>Isotope</th>
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<th>30days</th>
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<th>360days</th>
<th>30days</th>
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</thead>
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<tr>
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<td>$2.23 \times 10^{-5}$</td>
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</tbody>
</table>

Table 3.6: Production of noble gases for each reactor design. All numbers represent atom density in units of $\text{atoms/(barn \cdot cm)}$. The row labeled ‘Ternary f.’ is the fraction of $^4$He produced by ternary fission, as distinct from that produced by $\alpha$-decay. The reactor was kept running at constant power for a year, and was then down for another year.
Table 3.7: Total mass (g/cm³) of uranium and plutonium, and burnup (GWd/tHM) at each burn step. The reactor was kept running at constant power for a year, and was then down for another year.
4 BURNUP ANALYSIS OF TRISO FUEL

4.1 Introduction

Besides fission gases, other isotopes such as cesium, silver, iodine, strontium, etc., produced during fuel burnup are important to TRISO fuel performance analysis, because these isotopes are known to be highly penetrating and they might cause radioactivity leakage. Another fission product, palladium, is known to be reactive with SiC and thus decreases the strength of the SiC layer [17, 21]. Analysis of how these isotopes transport through the fuel and coating layers can not be carried out without knowing how much of each is produced. Burnup calculation can not only quantify the mass and activity change of these and other important isotopes such as fissile and fertile isotopes, but also track the change in the fuel reactivity. So burnup calculation provides important information for fuel performance analysis.

During burnup process, the nuclear fuel isotopic concentrations vary over time and space, and so does neutron flux and energy spectrum. So, for burnup analysis one has to solve the coupled equations of time- and space-dependent isotopic concentration and the static multigroup neutron diffusion equation or the transport equation. The changes in isotopic concentration cause changes in macroscopic neutron cross-section and thus cause changes in the neutron flux, which then affects the rate of change in the isotopic concentration. In general, core thermal-hydraulic also impacts burnup studies since the neutron cross-section is temperature-dependent. In practice, the flux is assumed to be constant over time intervals, and thus the two sets of equations are decoupled, and the depletion equation can be solved. At the end of each time interval, the updated densities (the results of depletion calculation) are used to solve the multigroup neutron diffusion equation or the transport equation to determine the neutron flux for
the next time interval. For neutron flux and energy spectrum calculation of one time
and small size problems, Monte Carlo method has gained more popularity over dif-
fusion methods, because Monte Carlo method takes advantage of continuous neutron
energy cross section and full 3D geometry while diffusion method requires grouping
neutron cross section and simplification of geometry. The downside of Monte Carlo
method is that it requires much more intensive computation. Due to the ever improving
computing technology, Monte Carlo codes can now be run at reasonable computational
costs. There are a few Monte Carlo nuclear transport codes developed over the years,
including MCNP5/X, GEANT, KENO, TRIPOLI, etc. For the isotopic concentration
calculation, one has to solve the reaction rate of each reaction type deemed important
for each nuclide and the inter-connected decay chains among nuclides. There are two
main nuclide inventory codes: ORIGEN and CINDER, developed at Oak Ridge Na-
tional Laboratory and Los Alamos National Laboratory, respectively. ORIGEN uses
a matrix exponential method to solve a large system of coupled, linear and first-order
ordinary differential equations with constant coefficients, and it uses one-group neutron
energy cross section; CINDER uses Markovian chains to determine temporal densities
of nuclides in a radiation environment, solving for independent contributions to atom
densities in each of a number of linear nuclide chains, and it uses 63-group neutron
energy cross section.

There are several codes developed for burnup calculation, such as Monteburns [50],
SCALE [51], MOCUP [52] and MCNPX 2.6.0 [37]. They all use the state-of-art
MCNP5 or MCNPX for nuclear transport calculation except for SCALE, which uses
a different Monte Carlo code named KENO. MCNPX 2.6.0, developed at Los Alamos
National Laboratory, was chosen for our calculation because MCNPX 2.6.0 includes
CINDER’90 for nuclide inventory calculation while the other codes link ORIGEN.
CINDER’90, with a vast database tracking 3400 nuclides, uses 63 neutron group cross
section while ORIGEN uses only one group. MCNPX 2.6.0 shows good agreement
with experiment on the mass of a number of important isotopes [53].

MCNPX 2.6.0 integrates CINDER’90 into the MCNPX Monte Carlo radiation trans-
port code to provide a completely self-contained Monte Carlo-linked depletion ca-
Fig. 4.1: Flow chart of the iteration between MCNPX and CINDER’90 for burnup calculation [53].

Fig. 4.1 shows the flow chart of the iteration between MCNPX and CINDER’90 [53]. As shown in this figure, MCNPX calculates neutron fluxes and CINDER’90 calculates isotopic number densities. During each time step, both neutron flux and isotopic number densities were assumed unchanged.
4.2 The burnup calculation model

A burnup analysis model was developed to track isotope creation and depletion inside a TRISO particle during irradiation time using the burnup capability in MCNPX 2.6.0. A “burn card” was added to the MCNPX input file to form a complete self-contained file to dictate both neutron transport and nuclide inventory calculation. The “burn card” consists of entries like burn time step, power fraction for each step, power for each material, material number, material volume, “BOPT”, etc. “BOPT” comprises options for output format control, fission product set and neutron cross section selection, etc. This burn model uses the same geometry as the heat generation model in chapter 2. Since there are thousands of TRISO particles packed inside a pebble ball, Body-Centered-Cubic (BCC) (unit-cell) is used to represent one TRISO with its 8 neighbors in an average sense. Pitch among particles is determined from the packing fraction. The kernel and the 4 coating layers of a TRISO are modelled explicitly. Reflective boundary conditions at all outer surfaces were assumed. Fig. 4.2 shows a TRISO with its neighbors. Gaps among the particles are filled with graphite.

The total power of this unit-cell model is assumed to be 59.2 mW or 24.6 mW per TRISO, which is equivalent to 1 kW per pebble – close to the mean power proposed for VHTR [35]. This burnup calculation uses 36 time steps and the final burnup of the
fuel is 72.8 GWd/tU (or 1,500 Equivalent Full Power Days (EFPD)), which is a little higher than the target of 65 GWd/tU for once-through fuel cycle [8]. There is a 30-day down time for maintenance every 400 days. The first and second time step after the reactor starts are 1.3 and 23.7 days to allow the reactor to achieve xenon and samarium equilibrium, respectively. The other time step is 50 days, or \( \sim 2.5 \) GWd/tU of burnup per step. Burnup calculation is computationally intense. More time steps require more Monte Carlo runs and thus higher computational load. On the other hand, the longer a time step is, the less accurate the results are, because the isotopic composition may change dramatically during a long time step rather than relatively constant as assumed. The current time step choice is optimal with consideration of both of these factors [52]. Each Monte Carlo run tracks 1.5 million particle histories. This burnup calculation took 17 days to complete on a 64-CPU cluster (4 GB memory on each node).

4.3 Burnup results

**Fig. 4.3** shows the effective multiplication factor \( (k_{\text{eff}}) \) as a function of both burnup and Equivalent Full Power Day (EFPD). As shown, \( k_{\text{eff}} \) starts around 1.1 and drops to 0.81 at the burnup of 72 GWd/tU. It drops below 1.0 after 275 EFPD days or 13.3 GWd/tU. It means that the reactor can not run beyond 275 days without refuelling. The current design of pebble bed reactor uses online refuelling, so this problem can be mitigated. Other ways to increase the interval between refuelling are: 1) to increase fuel enrichment; 2) to increase packing factor of TRISO. Both approaches will increase fissile materials in unit volume.

**Fig. 4.4** shows the mass of \( \text{235U}, \text{238U}, \text{239Pu} \) and \( \text{241Pu} \) in a TRISO as a function of burnup and EFPD. As expected, \( \text{235U} \) and \( \text{238U} \) decrease with burnup while \( \text{239Pu} \) and \( \text{241Pu} \) increase with burnup. \( \text{241Pu} \) grows at a slower rate than \( \text{239Pu} \) since it takes 2 more extra steps for \( \text{238U} \) to be converted to \( \text{241Pu} \). **Fig. 4.5** shows the variation of conversion ratio, defined as the ratio of fissile atom production rate to fissile atom consumption rate [36], of TRISO fuel as a function of burnup. As shown, the conversion ratio increases
Fig. 4.3: $k_{\text{eff}}$ as a function of both burnup (GWd/tU) and Equivalent Full Power Days (EFPD).

Fig. 4.4: The variation of $^{235}\text{U}$, $^{238}\text{U}$, $^{239}\text{Pu}$ and $^{241}\text{Pu}$ mass in a TRISO as a function of both burnup (GWd/tU) and Equivalent Full Power Days (EFPD).
Fig. 4.5: The variation of conversion ratio of TRISO fuel as a function of burnup (GWd/tU).

with burnup. Note that the “irregularities” on some curves as shown in this figure and some other figures in this chapter were caused by discontinuities in burnup history (30-day down time every 400 days) and were also because some isotopes have relatively short half-time. As expected, the conversion ratio of TRISO fuel is mostly higher than that of light water reactor (~0.6) mainly because of less neutron absorption in graphite than in water. Higher conversion ratio was observed at higher burnup, because there are more $^{239}$Pu and $^{241}$Pu at higher burnup (as shown in Fig. 4.4) and they produce more neutrons per unit mass than $^{235}$U, and thus convert more $^{238}$U into Pu.

Fig. 4.6 shows the production of xenon, krypton and helium (mol) as a function of both burnup and Equivalent Full Power Days (EFPD). As shown, the total production of xenon is approximately one order of magnitude higher than that of krypton, and two orders of magnitude higher than $^4$He. The reason why these gases were quantified in terms of molar unit is because the specific pressure buildup caused by each gas is proportional to its molar quantity. So xenon contributes to most of the pressure buildup.
Among them, $^{134}$Xe and $^{136}$Xe are two most important isotopes contributing to pressure buildup.

Palladium, as one of the fission products, is known to react with silicon-carbide (SiC) to form compound Pd$_2$Si [21] that has less mechanical strength, and thus degrades the integrity of the SiC layer. Fig. 4.7 shows the production of palladium isotopes as a function of burnup. As shown, the total Pd produced is of the order of 1E-6 mol at the end of burnup, with $^{105}$Pd as the most abundant isotope.

Silver is also one of the fission products, which is known to have high penetrability. $^{110}$Ag, a metastable isotope, can migrate out of the coatings of the TRISO particle and can cause radioactivity leakage. Fig. 4.8 shows the production of $^{110}$Ag (mol/THM) as a function of burnup. The results agree well with the results reported in literature [17].

$^{134}$Cs, $^{137}$Cs, $^{90}$Sr and $^{95}$Zr are major fission products which emit gamma radiation. Fig. 4.9 shows the mass of each of these four isotopes produced in a TRISO particle as a function of burnup. Fig. 4.10 shows the mass ratio of $^{134}$Cs to $^{137}$Cs as a function of
Fig. 4.7: Production of palladium as a function of both burnup and Equivalent Full Power Days (EFPD)).

Fig. 4.8: Production of $^{110}\text{Ag}$ (mol/tHM) as a function of both burnup and Equivalent Full Power Days (EFPD). Discontinuities in the curve are due to discontinuities in the burnup history.
Fig. 4.9: Mass of $^{134}$Cs, $^{137}$Cs, $^{90}$Sr and $^{95}$Zr (gram) produced in a TRISO as a function of burnup. (Discontinuities in the curve for $^{95}$Zr are due to 30-day downtime in the burnup history since $^{95}$Zr has a relatively short decay half-time ($T_{1/2} = 64$ days).)

Fig. 4.10: Isotopic ratio of $^{134}$Cs to $^{137}$Cs as a function of burnup.
Fig. 4.11: Activity (Ci) of $^{134}$Cs, $^{137}$Cs, $^{90}$Sr and $^{95}$Zr in a TRISO as a function of burnup. (The sharp change on the curve of $^{134}$Cs and $^{95}$Zr are due to the fact that the MCNPX code stops tracking when the mass of certain isotope falls below some cutoff value.)

Fig. 4.12: Activity (Ci) of $^{134}$Cs, $^{137}$Cs, $^{90}$Sr and $^{95}$Zr in a TRISO as a function of burnup.
Fig. 4.13: Neutron energy spectrum in TRISO kernel at four different burnups. As shown, the ratio increases steadily with burnup. (Again, the discontinuities are due to discontinuities in burnup history.) This ratio is used in nuclear safeguard field to measure burnup of target spent fuel [54]. Fig. 4.11 shows the radiation activity (Ci) of each of the four isotopes ($^{134}\text{Cs}$, $^{137}\text{Cs}$, $^{90}\text{Sr}$ and $^{95}\text{Zr}$). As shown, $^{95}\text{Zr}$ is the dominant radiation source. Fig. 4.12 shows the radiation activity of each of these four isotopes as a function of cooling time. As shown, $^{95}\text{Zr}$ decays off very quickly after reactor shuts down, and $^{134}\text{Cs}$ decays off after 7,000 days. $^{137}\text{Cs}$ and $^{90}\text{Sr}$ remain the long-term radiation source.

4.4 Neutron energy spectrum and fast neutron fluence

Fig. 4.13 shows neutron energy spectrum in the TRISO kernel at four different burnups. For all burnups, the neutron energy spectrum is relatively hard compared to light water reactor, and the reason is two-fold: the initial enrichment of the fuel is relatively high (14%) and thus there are large absorption occurring at thermal energies; graphite is a
less efficient neutron moderator than water [54]. The main difference in the spectrum among the four different fuels are at the neutron energy below 1 eV (especially in the neighborhood of 0.3 eV)–higher burnup fuel has lower neutron flux in this energy range. There are more $^{239}$Pu and $^{241}$Pu at higher burnup (as shown in Fig. 4.4), and they both have higher fission and absorption cross section than $^{235}$U (in particular, there is a resonance fission and absorption cross section for both $^{239}$Pu and $^{241}$Pu at the energy of 0.3 eV). The higher neutron cross section in higher burnup fuels leads to more neutron absorption and thus depress the neutron flux in this energy region ($< 0.1$ eV).

Fast neutron flux irradiation can cause a lot of changes in nuclear fuel and shielding materials, such as atom displacement and vacancies in the atomic lattice. The accumulated flux is measured as fast neutron fluence, which has been widely used as a parameter to evaluate the accumulated impact of fast irradiation on material performance. For instance, fast neutron fluence is used as an input parameter for the thermal conductivity model of the fuel as described in Chapter 2, and it is also used in the irradiation creep model of pyrocarbon. Table 4.1 shows the neutron flux and fast neutron fluence in the kernel of a TRISO at different burnup. Neutrons with energy above 0.18 MeV are referred to as fast neutrons here. As shown, fast neutrons represent $\sim 28\%$ of the total neutron population in the fuel. Fast neutron fluence reaches above $5.33 \times 10^{25}$ n/m$^2$ at the end of burnup (73 GWd/tU). Fig. 4.14 shows the fast neutron fluence as a function of burnup. As can be seen, the fast neutron fluence increases almost linearly with burnup. Since the size of a TRISO particle is so small compared to the mean free path of the coating materials, (for example the mean free path of graphite is $\sim 2.6$ cm,) the neutron flux in the coating layers are very similar to that in the kernel. Further calculations also show that less than 1% difference in either neutron flux or fast neutron fraction is found between the kernel and outer layers. Hence, fast neutron fluence obtained for kernel can also be applied to outer layers.

In summary, these burnup results provide valuable dataset for nuclear engineers and material scientists who are designing the reactor core or evaluating fuel performance as a function of fuel burnup. The results presented in this chapter indicate how the internal gas pressure (gas production), the radioactivity, the fast neutron fluence and the rate of
Burnup total flux fast flux, EFPD fast fluence 
\((GWd/tU) (n/(cm^2 - s)) \% \) (days) \((n/m^2)\) 

<table>
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<th>total flux (n/(cm^2 - s))</th>
<th>fast flux, %</th>
<th>EFPD () days</th>
<th>fast fluence (n/m^2)</th>
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<tr>
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<td>28.0a</td>
<td>1,500t</td>
<td>5.33E25t</td>
</tr>
</tbody>
</table>

Table 4.1: Neutron flux and fast neutron fluence \((E > 0.18 MeV)\) in TRISO kernel at different fuel burnup range. \(\ast\): “t” stands for total and “a” stands for average.

Fig. 4.14: Fast neutron fluence \((\times 10^{25} \text{ n/m}^2)\) as a function of burnup in TRISO kernel.

Pd production change with burnup, which are important input parameters for the stress and failure analysis.
5 FISSION GAS RELEASE AND INTERNAL GAS PRESSURE BUILDUP IN TRISO PARTICLE

5.1 Introduction

Fission gas release is of significant interest in TRISO fuel safety analysis. For example, the fraction of gas release from the fuel kernel into the buffer layer dictates the pressure buildup in the buffer layer, which then affects the stress state of the TRISO particle. To evaluate the deleterious nature of gas release requires a detailed knowledge of how gases migrate on intra- and inter-granular level. In this chapter, the fractional release of gases from fuel kernel is estimated using the improved Booth model proposed by White and Tucker [55]. The internal gas pressure buildup in the buffer layer is also estimated under various assumptions.

5.2 Fractional release from the fuel kernel

5.2.1 The Booth model and the White and Tucker model

A number of models have been developed by previous researchers to predict the fractional release of stable gases from the fuel (mainly UO$_2$). Booth [56] developed one of the earliest models, in which the fuel grains are approximated by so-called equivalent spheres. Atomic gases diffuse through the sphere, and the boundary is treated as a perfect sink. Speight [57] improved the perfect sink assumption by introducing two parameters: the resolution layer depth and probability of grain boundary gas returning back into grains. Turnbull [58], White and Tucker [55], Rest [59], and Forsberg and Massih [60] carried the work forward.

Although significant disagreements exist in literature over the details of the complex
gas release, it is generally agreed that the gas release can be reduced into two stages. In the first stage, gas atoms are produced inside grains and then migrate by several mechanisms towards the grain boundaries. Intragranular bubbles are nucleated in the wake of energetic fission fragments and they grow by collecting more gas atoms. At the same time these bubbles can be destroyed by the passage of other fission fragments. Bubbles are continuously created and destroyed by this precipitation and re-solution process inside the grains. In the second stage, on grain boundaries larger bubbles are formed, grow, and finally inter-link each other. Once an open-tunnel network is established along the grain boundaries, the accumulated gases are released immediately to free volume (the porous buffer layer in this case). On the other hand gas atoms in these bubbles can also diffuse back into the grains. Right before the release, a saturation concentration on grain boundaries is assumed to be met. This is the so-called incubation time, which is also observed in experiment (i.e., gas was not released till certain burnup was achieved). After that, the tunnel diminishes and then the whole process starts over and repeats itself.

Based on this theory, White and Tucker modified the classic Booth model to include new physics such as intragranular absorption and resolution etc. The White and Tucker model was adopted in an European fuel performance code—MINIPAT [61], and it is also adopted in this work because of its maturity.

5.2.2 Intragranular fractional release

The White and Tucker model starts with the Booth model, in which the polycrystalline fuel is viewed as a collection of uniform spheres of grains, or so-called equivalent spheres. The hypothetical sphere radius is defined as the effective surface-to-volume ratio of the fuel \((R = 3V/S)\), with \(R, V, S\) being radius, volume and surface, respectively. The gas concentration inside the equivalent sphere follows Fick’s law:

\[
\frac{\partial C(r,t)}{\partial t} = D(t)\Delta r C(r,t) + \beta(t),
\]

(5.1)
where \( C(r,t) \) is gas concentration, \( D(t) \) is the single gas atom diffusion coefficient, \( \beta(t) \) is gas generation rate, and \( \Delta_r \) is the Laplacian operator in spherical geometry,

\[
\Delta_r \equiv \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r}.
\] (5.2)

In the Booth model, *perfect sink* boundary is assumed (i.e., once the gas atom migrates to the grain boundary, it is completely released immediately). So the boundary and initial conditions are as follows:

\[
C(r,0) = 0, \quad C(R,t) = 0, \quad \frac{\partial C}{\partial r} = 0 \text{ at } r = 0.
\] (5.3)

Analytical solution for \( C(r,t) \) can be obtained, and the fraction of released gas, \( f_c(t) \) (defined as the release to birth rate ratio), is shown as below [55]:

\[
f_c(t) = 1 - 6 \sum_{n=1}^{\infty} \frac{1 - \exp(-\pi^2 n^2 \omega)}{(n\pi)^4},
\] (5.4)

with \( \omega \equiv Dt/R^2 \).

According to White and Tucker [55], the single gas atom diffusion coefficient, \( D \), has three components, \( D_1 \), \( D_2 \), and \( D_3 \), each reflecting the contribution of a specific migration mechanism to the overall diffusivity.

\[
D = D_1 + D_2 + D_3,
\] (5.5)

where \( D_1 \) is the contribution of the “intrinsic” thermally activated process dominating at higher temperatures; \( D_2 \) represents the diffusion by means of vacancies produced by the irradiation process below 1400°C; and \( D_3 \) represents the “athermal tail” of diffusion at lower temperatures that is proportional to fission rate. More details about \( D_1 \), \( D_2 \), and \( D_3 \) can be found in Ref. [55].

As discussed earlier there exists intragranular absorption and resolution due to intragranular bubbles. The single gas atom diffusion coefficient \( D \) can be adjusted to
account for the absorption and resolution [55]:

\[
D' = \frac{Db'}{(b' + g)},
\]  

(5.6)

where \(D'\) is the effective diffusion coefficient, \(b'\) and \(g\) are the intragranular resolution and absorption rate, respectively.

Based on the aforementioned assumptions, \(D\) and \(D'\) can be calculated. The value of \(D\) and \(D'\) at three selected temperatures are listed in Table 5.1 [55].

<table>
<thead>
<tr>
<th>Temp. (°C)</th>
<th>(D ) (m(^2)/s)</th>
<th>(D') (m(^2)/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>(7.98 \times 10^{-21})</td>
<td>(7.70 \times 10^{-21})</td>
</tr>
<tr>
<td>1200</td>
<td>(4.49 \times 10^{-20})</td>
<td>(3.82 \times 10^{-20})</td>
</tr>
<tr>
<td>1400</td>
<td>(6.32 \times 10^{-19})</td>
<td>(2.02 \times 10^{-19})</td>
</tr>
</tbody>
</table>

Table 5.1: Single atom diffusion coefficient \(D\) and the effective diffusion coefficient \(D'\), which accounts for intragranular absorption and resolution, at selected temperatures [55].

Replacing \(\omega\) by \(\omega'\) (\(\omega' = D't/R^2\)), the fraction of gas released from fuel grains can be calculated using Eq. 5.4. Fig. 5.1 shows the fraction of gas released from fuel grains as a function of irradiation time at three different temperatures (1000, 1200 and 1400°C). The radius of an average grain is assumed to be 5 \(\mu\)m. As shown, the fractional release is highly temperature dependent and release fraction is higher at higher temperature. Burnup reaches 65.5 GWd/tU around day 1350. There is no incubation time predicted by this model because it does not include the intergranular bubbles. The fraction increases rapidly initially and approaches close to 100% at high burnup in the 1400°C case.

5.2.3 Intergranular fractional release

The fractional release calculated in the previous subsection does not consider the intergranular bubbles, and it essentially describes only the first stage. Further modifications were proposed by White and Tucker to include the second stage of gas release from
Fig. 5.1: Fraction of gas released on intragranular level as a function irradiation time, at three different temperatures.

The fuel. First they developed a model to predict the maximum number of gas atoms per unit area of grain surface (saturation density, $N^m$), based on the balance of internal bubble pressure and the capillary forces restraining the bubble in addition to external forces [55]:

$$N^m = \frac{4V_c f(\theta)r}{3k_B T \sin^2 \theta} \left( \frac{2\gamma}{r} + P_{\text{ext}} \right), \quad (5.7)$$

where $r$ is bubble radius, $\gamma$ is bubble surface tension, $k_B$ is Boltzmann constant, $T$ is temperature, $V_c$ is the fraction of the grain surface occupied by the bubbles at saturation, $P_{\text{ext}}$ is externally applied hydrostatic pressure, and $f(\theta)$ is a factor to account for the deviation of the bubble shape from spherical (these bubbles on the grain boundaries are usually lenticular-shaped). It is defined as $f(\theta) = 1 - 3 \cos \theta/2 + \cos^3 \theta/2$. More details of $\theta$ can be found in Ref. [62]. For a spherical bubble, $\theta = 90^\circ$, and for a lenticular bubble in this case, $\theta$ is assumed to be $50^\circ$.

When the area atom density $N$ approaches $N^m$, the accumulation of gases at the grain boundary is assumed to be saturated, and the time it takes to get to this point is called
the incubation time ($t_{inc}$). Prior to saturation, the fractional release can be calculated by [62]:

$$f_{c1} = 3\phi N^m / 2a \beta t,$$

(5.8)

where $\phi = N / N^m$, $a$ is average bubble radius, $\beta$ is gas atom generation rate, and $t$ is irradiation time.

At saturation, as suggested by Speight [57] and Olander [20], an equilibrium condition should be reached within the resolution layer of a grain (a layer in a grain adjacent to the grain boundary with small thickness (resolution depth, $\delta$)), when the local diffusion flux (from grain to grain boundary) balances the resolution flux (from grain boundary bubble to grain). White and Tucker further developed this model and proposed that [55]:

$$\phi = A \left( u^2 - 2u + 2 - 2e^{-u} \right), \quad \text{with } A = \frac{\beta \pi D'^2}{8(b\delta)^3 N^m}, \quad \text{and } u = \frac{4b\delta \sqrt{t}}{\sqrt{D' \pi}},$$

(5.9)

where $b$ is resolution probability. Incubation time ($t_{inc}$) can be solved using this equation when $\phi(t = t_{inc}) = 1$. Since this is an implicit equation for $t$, an iterative process is required to find this particular time ($t_{inc}$). Because most of the gas atoms migrating to the grain boundaries are stored in the grain boundary bubbles, no significant gas release is observed from fuel during incubation period. Table 5.2 shows the incubation time in terms of irradiation time (days) and burnup (GWd/tU) at three different temperatures. The incubation time ranges from $\sim$8 days to $\sim$80 days at temperature from 1000 to 1400°C. As expected, temperature has a major impact on incubation time, and the incubation time is lower at higher temperature. (Values of a few parameters used in calculations reported in this section are listed in Table 5.3. Some of them are taken as the mid point value from the range suggested by Ref. [62].)

After saturation, it is assumed that all gas arriving at grain boundaries would be released immediately because the grain boundaries are saturated already. So the fractional release after saturation, $f_{c2}$ has two parts: 1) the release from the grain to grain boundaries as determined by intragranular $f_c$ as described in the previous subsection;
Table 5.2: Incubation time of gas release from grain boundary in terms of irradiation time (days) and burnup (GWd/tU) at three different temperatures.

<table>
<thead>
<tr>
<th>Temp. (°C)</th>
<th>incubation time (t_{inc})</th>
<th>irradiation (days)</th>
<th>burnup (GWd/tU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td></td>
<td>79.9</td>
<td>3.88</td>
</tr>
<tr>
<td>1200</td>
<td></td>
<td>21.5</td>
<td>1.04</td>
</tr>
<tr>
<td>1400</td>
<td></td>
<td>8.5</td>
<td>0.41</td>
</tr>
</tbody>
</table>

Table 5.3: List of parameters used in calculations reported in this section [62].

2) the release from the grain boundary bubbles. The fractional release of the second part, $f_{c'}$, can be calculated as [58]:

\[
f_{c2} = f_c + f_{c'}, \quad \text{with}\]
\[
f_{c'} = 4 \left( \frac{D' t}{\pi a^2} \right)^{1/2} - 3 D' t + \frac{C^0 - C^m}{\beta t} \left[ 6 \left( \frac{D' t}{\pi a^2} \right)^{1/2} - 3 D' t \right],
\]

where $C^0$ is the gas atom concentration at saturation, expressed as: $C^0 = \beta_{inc} - 3 N^m / 2a$. $C^m$ is the effective grain-boundary gas concentration, expressed as: $C^m = b \delta N^m / 2D'$ [62].

With these equations, the fractional release on intergranular level, which is considered equivalent to release from the kernel to the buffer layer, before and after saturation are calculated. Fig. 5.2 shows the fraction of gas released on intergranular level as a function of irradiation time (days) and burnup (GWd/tU) at three different temperatures. As expected, the release fraction is low before saturation and there is a dramatic
Fig. 5.2: Fraction of gas released on intergranular level as a function of irradiation time (days) and burnup (GWd/tU) at three different temperatures.

Increase after saturation. At higher temperature, it takes less time to reach saturation and the release fraction is higher. At 1400°C, the release fraction approaches 1.0 around day 180, which means an open-tunnel network along grain boundaries leading to free volume has been established and remains open after that. For the two lower temperatures (1000 and 1200°C), such a situation might not occur within a single fuel cycle. In Ref. [17], it is reported that the release fraction is 0.23 at 900°C with medium burnup, and 0.86 at 1200°C with high burnup predicted by the PARFUME fuel performance code. The agreement between this work and the reference is deemed acceptable, given that a lot of details were not included in this reference.

5.3 Internal gas pressure buildup

It is important to quantify the internal gas pressure buildup in the buffer layer because it is an important input to evaluate the stress state of the other coating layers. The ideal
gas law is used to calculate the pressure:

\[ P = \frac{n_f c_2 RT}{V_b p_0}, \]

(5.12)

where \( P \) is pressure (Pa); \( n_f \) is the total molar quantities of all gases produced in a TRISO particle at certain burnup (mol); \( f_{c2} \) is fraction of the gas released from the kernel into the buffer layer, as discussed in the previous section; \( V_b \) is the volume of the buffer layer (m\(^3\)); and \( p_0 \) is the porosity of the buffer layer. The total molar quantities of all the gases (Xe, Kr and He) are discussed in the previous chapter. The release fraction, \( f_{c2} \), of gases from the kernel to the buffer layer is calculated in the previous section.

As shown in Fig. 5.2, \( f_{c2} \) varies dramatically at different temperature and burnup. The exact porosity of the buffer layer is not known and it is assumed to be in the range of 0.2 to 0.4 [17]. Given the variation of a number of parameters, the exact pressure in the buffer layer is difficult to determine. Hence, a range is determined for pressure using high-end and low-end values of these parameters. Two extreme porosities, 0.2 and 0.4; two extreme release fractions, 0.25 and 1.0; and two extreme operating temperatures, 800 and 1200°C are used in this calculation. The pressure in the buffer layer at the burnup of 72.78 GWd/tU (or irradiation time of 1500 days) is shown in Table 5.4. As shown, the pressure varies from 2.24 to 24.6 MPa. In the stress analysis reported in the next chapter, a smaller burnup range (0−41.4 GWd/tU), within which the stress analysis is performed, is determined to be sufficient with reasons specified in the next chapter. To obtain conservative results on failure prediction, a high-end gas pressure, 15.75 MPa, is used for most cases, and the sensitivity of stresses to the pressure is also studied.

In summary, in this chapter, the process of gas migration out of the fuel (the kernel) is examined and the fractional release of gas on both intra- and inter-granular level is calculated with the White and Tucker model. The range of the gas pressure in the buffer layer is also determined. The pressure is an important input parameter for the stress analysis discussed in the next chapter.
<table>
<thead>
<tr>
<th>Porosity (po)</th>
<th>release fraction ($f_{c2}$)</th>
<th>temperature (°C)</th>
<th>pressure (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.25</td>
<td>800</td>
<td>4.49</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1200</td>
<td>6.16</td>
</tr>
<tr>
<td>0.2</td>
<td>1.0</td>
<td>800</td>
<td>17.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1200</td>
<td>24.6</td>
</tr>
<tr>
<td>0.4</td>
<td>0.25</td>
<td>800</td>
<td>2.24</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1200</td>
<td>3.08</td>
</tr>
<tr>
<td>0.4</td>
<td>1.0</td>
<td>800</td>
<td>8.97</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1200</td>
<td>12.3</td>
</tr>
</tbody>
</table>

Table 5.4: Pressure in the buffer layer based on various assumptions at the burnup of 72.78 GWd/tU (or irradiation time of 1500 days).
6 STRESS MODEL DEVELOPMENT AND SIMULATION AND FAILURE PREDICTION FOR TRISO PARTICLES

6.1 Introduction

During irradiation, a TRISO particle experiences complex stress states induced by thermo-mechanical processes. These processes are well reported in literature [20]. For example, fission gases accumulate inside the kernel and the buffer layer, and build up internal pressure. The pyrolytic carbon (PyC, also called pyrocarbon), in both IPyC and OPyC layers, is known to experience dimensional changes (shrinkage or swelling) under fast neutron irradiation [14, 15, 17, 63]. In the mean time, both IPyC and OPyC layers creep as a function of stress and fast neutron fluence [15, 17, 19, 20, 64]. Macro cracks in the IPyC layer, corrosion in the SiC layer due to chemical attack, and debonding at the interface between IPyC and SiC have been observed in post-irradiation examination [7, 13]. All of these processes/conditions further complicate the stress states. In order to predict the stress states in the coating layers and to ensure the coating layers, especially the SiC layer (the strongest layer), maintain their mechanical integrity under different conditions, a comprehensive stress analysis is needed. All these aforementioned processes and conditions need to be included in this stress analysis, which has to be multi-dimensional, and must account for multiple physics, given the nature of the problem.

Most of the previous work found in literature on the TRISO stress analysis used the conventional pressure vessel model [12, 63, 65, 66], in which the coating layers were assumed to be “thin shell”, and thus the stresses in each layer were uniform and could be calculated using some simple relations. The particle fails when the stress in SiC layer exceeds its maximum strength. The pressure vessel model, as a single-physics and one-dimensional model, is not adequate because it over-simplifies the problem.
and does not account for the multi-physics, multi-dimensional nature. As a result, the pressure vessel model significantly underestimates the failure percentage observed in the NP-MHTGR fuel as well as other coated fuel designed in the United States [13,17].

Miller et al. developed a rather comprehensive stress model for TRISO fuel using the Abaqus code [13,67]. The fact that Abaqus, as a commercial code, does not offer users the access to its source code makes it difficult for the users to add new capabilities to the code. Costly annual license fees are an additional drawback of multi-purpose commercial finite element codes like Abaqus. Given the complex nature of the TRISO particle stress analysis and the unusual material properties, e.g., the irradiation-induced shrinkage of pyrolytic carbon, an open-source finite element code is a better fit for this problem. In this work, the open-source finite element code–FEAP [27] is chosen to conduct the stress analysis of a TRISO particle. FEAP is a general purpose, well benchmarked and multi-dimensional finite element analysis program which is designed for research and educational use. Source code of the full program is available for compilation using Windows, LINUX or UNIX operating systems, and Mac OS X based Apple systems [27]. FEAP was developed at the University of California, Berkeley, and it is actively maintained and constantly updated. In addition to the fact that users can customize the code according to their specific needs with the full access to the source code, FEAP also offers the feature of “user material models” which makes it convenient for users to define new material models to include new physics. In this work, new user material models for both irradiation-induced dimensional change and creep are included. The source code is also modified to include time-dependent convective heat transfer boundary conditions.

New stress models are developed using FEAP (with added capabilities) and the results are presented in the following sections. Given that the buffer layer is made of porous carbon with low density and low mechanical strength, it is determined sufficient to include only the outer three coating layers (namely IPyC, SiC and OPyC) in the stress model. The impact from the kernel and the buffer layer is accounted for by applying a pressure and thermal boundary condition on the inner surface of the IPyC layer.
6.2 Material properties of PyC and SiC

A stress model cannot be built without knowing the material properties of the TRISO particle. These properties usually vary with a number of variables such as temperature, density, anisotropy (measured by Bacon Anisotropy Factor\(^1\) (BAF)), fast neutron fluence (or burnup), etc. (Note that neutron fluence used in this chapter always means fast neutron fluence with neutron energy above 0.18 MeV.) The property data of material exposed to high neutron fluence and high temperature is generally scarce. Also significant scatter has been observed for some properties among different sources. Uncertainties in material properties introduce significant uncertainties in model prediction of stresses and probability of failure. Fortunately, the CEGA corporation compiled a report on the coated particle material properties based on historical values found in open literature [15]. Some correlations were also developed in that report using empirical fittings. A few properties key to the stress analysis are discussed below. Note that both IPyC and OPyC layers use the same material pyrocarbon (PyC). Irradiation-induced shrinkage and creep in SiC are much lower in magnitude than that in PyC [15], therefore they are not considered in this work.

6.2.1 Elastic modulus (E), Poisson ratio (v), CTE (\(\alpha\)), and \(T_0\)

The Elastic modulus (E) of Pyrolytic carbon depends primarily on neutron fluence since the dependence on temperature, density or BAF are weak [15]. The modulus increases from 21 to 37 GPa when the neutron fluence changes from 0 to \(3 \times 10^{25} \text{ n/m}^2\) [69]. The original FEAP implementation does not include a time-dependent elastic modulus and later research shows that varying the value of the modulus in this range has minor impact on the stresses. So, an average value, 29 GPa, is used in this work. The Elastic modulus of SiC, as a brittle material, has a significant scatter in literature. The modulus decreases with temperature and it also varies due to inherent variability caused by de-

\(^1\)Bacon Anisotropy Factor is used to represent the degree of preferred orientation of PyC [68], which is usually quantified as the ratio of the thermal expansion coefficient in two different directions (normal and parallel to the deposition plane) at 400°C, and it is considered equivalent to the neutron expansion.
position condition, sample preparation, etc. The modulus value at \(\sim 800^\circ\text{C}\), 330 GPa, is used in this work.

The Poisson ratio \((v)\) of PyC and SiC are set as 0.33 and 0.13 respectively as recommended in the CEGA report [15].

Coefficient of thermal expansion (CTE, denoted by \(\alpha\)) is needed to evaluate the thermal stress induced by differential thermal expansion among the coating layers. Fig. 6.1 shows coefficient of thermal expansion (CTE) of PyC as a function of temperature [16]. An empirical fitting using second-order polynomial is developed in this work to fit this curve, and then the fitting function is included in the “user material models” in FEAP. The value of CTE at 780 K (or 507\(^\circ\text{C}\)) is used for all temperatures above 780 K. CTE of SiC is lower than PyC and it varies in a smaller range of \(4\times10^{-6}/^\circ\text{C}\), so the average value of \(4.5\times10^{-6}/^\circ\text{C}\) is used in this work.

The stress free temperature, \(T_0\), is set as the manufacturing temperature, 1200\(^\circ\text{C}\). Table 6.1 summarizes the material properties of PyC and SiC used in this work.

\[\text{Fig. 6.1: Coefficient of thermal expansion (CTE) of PyC as a function of temperature [16].}\]
<table>
<thead>
<tr>
<th>Item</th>
<th>PyC</th>
<th>SiC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic Modulus (GPa)</td>
<td>29</td>
<td>330</td>
</tr>
<tr>
<td>Poisson Ratio</td>
<td>0.33</td>
<td>0.13</td>
</tr>
<tr>
<td>CTE ($\times 10^{-6}/^\circ C$)</td>
<td>temp.-dependent</td>
<td>4.5</td>
</tr>
<tr>
<td>$T_0$ ($^\circ C$)</td>
<td>1200</td>
<td>1200</td>
</tr>
</tbody>
</table>

Table 6.1: The material properties of PyC and SiC used in this work.

6.2.2 Irradiation-induced dimensional change in PyC

Pyrocarbon is reported to experience dimensional change due to fast neutron irradiation [14, 15, 17, 63]. The rate of dimensional change is a strong function of irradiation temperature and initial anisotropy (BAF), although it also depends on initial density, crystallite size, etc. PyC shrinks (or swells) differently in the radial and tangential directions due to the anisotropy of the PyC layers. Given the significant scatter in data in literature, (and the precise attributes of PyC being unknown,) it is not possible to perform simple quantitative regression analysis to obtain a specific expression for dimensional change as a function of all variables.

Fig. 6.2 depicts the PyC radial and tangential strains as a function of fast neutron fluence ($\times 10^{25}$ n/m$^2$, $E > 0.18$ MeV) at 3 different irradiation temperatures (700, 910 and 1215$^\circ C$) [18, 24]. BAF is fixed at 1.08 in this case. In this figure, the markers represent experimental data found in the CEGA report. The fitting is a compromise between the CEGA data and the UK STRESS3 correlations [16]. Notice in Fig. 6.2(b) that there is an acceleration in the tangential strain after fluence of $4.0\times 10^{25}$ n/m$^2$, the cause of which is not well understood at this point. Significant uncertainties exist when neutron fluence is beyond $3.7\times 10^{25}$ n/m$^2$ [17]. Nevertheless, empirical functions are developed in this work based on the fits in Fig. 6.2. In radial direction (shown in Fig. 6.2(a)), PyC shrinks initially and then swells with neutron fluence; while in tangential direction (shown in Fig. 6.2(b), PyC shrinks continuously.

Fig. 6.3 depicts the PyC radial and tangential strains as a function of fast neutron fluence ($\times 10^{25}$ n/m$^2$, $E > 0.18$ MeV) with 4 different BAFs (1.02, 1.08, 1.17 and 1.28). In this figure, the markers represent data obtained from the INL report [24]. The
Fig. 6.2: Irradiation-induced strain (%) in PyC as a function of fast neutron fluence (×10^{25} \text{n/m}^2) at different irradiation temperature: (a) radial strain; (b) tangential strain [24].

As shown, PyC with higher initial anisotropy (BAF) has higher magnitude of strains in both directions. The dependence on BAF is significant.

Several second- or third-order polynomial correlations are developed to fit each curve in these two figures. A Fortran subroutine ‘shrink.f’ is written in this work to linearly interpolate among the 3 aforementioned temperature and 4 BAFs. With this subroutine, the radial and tangential strains of PyC with arbitrarily given BAF and temperature at certain neutron fluence can be calculated. To avoid introducing additional uncertainties, no extrapolation is allowed, i.e., when the temperature or BAF lies outside the preset range, strains at the closest within-range temperature or BAF will be used instead.

As a reference, Fig. 6.4 shows the shrinkage strains based on German FZJ and UK BNFL correlations [17]. All these three datasets (INL, FZJ and BNFL) fall into similar ballparks, although noticeable differences exist. Obviously more experimental shrinkage strain data at different temperatures, BAFs, or other attributes are needed to develop more conclusive correlations for the future, as indicated in a recent NEUP proposal call [40].
Fig. 6.3: Irradiation-induced strain (%) in PyC as a function of fast neutron fluence ($\times 10^{25}$ n/m$^2$) with different anisotropy (BAF): (a) radial strain; (b) tangential strain [24].

Fig. 6.4: Irradiation-induced strain (%) in PyC as a function of fast neutron fluence ($\times 10^{25}$ n/m$^2$) based on German FZJ and UK BNFL correlations [17].
6.2.3 Irradiation-induced creep in PyC

PyC is also known to creep under neutron irradiation and stress [15, 17, 19, 20, 64]. Creep is another important property of PyC that has a major impact on the stress state. The rate of creep strain mainly depends on fast neutron flux and stress, which can be predicted using the relation suggested by Price and Bokros [19] for uniaxial loading, as expressed below:

\[ \dot{\varepsilon} = K \sigma_e \Phi, \]  

(6.1)

where \( K \) is steady-state creep constant, \( \sigma_e \) is effective creep stress, and \( \Phi \) is the fast-neutron flux (\( E > 0.18 \) MeV) [64]. In 3D, this relation can be fully expressed as below:

\[ \dot{\varepsilon}_1 = K[\sigma_1 - \nu_c(\sigma_2 + \sigma_3)]\Phi, \]  

(6.2)

where \( \dot{\varepsilon}_1 \) is the creep strain rate in the first principal direction, \( \sigma_1, \sigma_2 \) and \( \sigma_3 \) are the principal stresses, and \( \nu_c \) is Poisson’s ratio in creep. Creep strain rate in the other two principal directions can be calculated accordingly. Creep is a relaxing mechanism that reduces stress caused by other mechanisms.

There is significant scatter in the creep constant (\( K \)) and creep Poisson ratio (\( \nu_c \)) of PyC as reported in literature. \( K \) varies from 1.0 to \( 4.9 \times 10^{-29} \) (MPa(n/m\(^2\)))\(^{-1} \) [15, 17]. \( \nu_c \) is quoted over a range of 0.3 to 0.5, it is generally acknowledged that a realistic value is closer to 0.4 [17, 25]. Based on historical values, an empirical relation for the creep constant, referred to as the CEGA correlation, was developed in the CEGA report [15]:

\[ K = K_{S0}(1 + 2.38(1.9 - \rho)), \text{ for } \rho < 2.05 \text{ g/cm}^3, \]  

(6.3)

where \( K_{S0} \) is the value of \( K \) at \( \rho = 1.9 \) g/cm\(^3\). \( K_{S0} \) mainly depends on irradiation temperature (\( T, ^\circ C \)):

\[ K_{S0} = 2.193 \times 10^{-29} - 4.85 \times 10^{-32} * T + 4.0147 \times 10^{-35} * T^2 \text{ (MPa(n/m}^2\text{)))}^{-1}. \]  

(6.4)

Table 6.2 lists the creep constant at 4 different temperatures calculated using Eq. 6.3
and Eq. 6.4. The density of PyC is set as 1.9 g/cm$^3$ in this work.

<table>
<thead>
<tr>
<th>Temperature ($T$, °C)</th>
<th>Creep constant ($K \times 10^{-29}$ (MPa(n/m$^2$))$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
<td>0.73</td>
</tr>
<tr>
<td>800</td>
<td>0.88</td>
</tr>
<tr>
<td>1000</td>
<td>1.36</td>
</tr>
<tr>
<td>1200</td>
<td>2.15</td>
</tr>
</tbody>
</table>

Table 6.2: Creep constant of PyC ($\rho = 1.9$ g/cm$^3$) at different irradiation temperature.

Miller et al. [17, 70] concluded that when the creep constant that is twice as large as that determined by this CEGA correlation, together with a creep Poisson’s ratio of 0.4, are used in stress models, the resulting failure predictions are in a better agreement with the observations made in the irradiation experiments of the NP-MHTGR program. Besides, this amplified creep constant is closer to what was used in older performance models developed in Europe [16]. In most part of this work (unless stated otherwise), twice of the CEGA value for creep constant and a creep Poisson’s ratio of 0.4 are used.

### 6.3 Code modifications and stress model development with FEAP

The finite element method (FEM) has evolved to a general technique for solving non-linear, transient, partial differential equations. A few FEM codes have been developed for mechanical analysis, especially for solid mechanics, over the years. Commercial codes such as Abaqus, ANSYS are widely used in industry. However, an open-source research FEM code is more suitable for this work because it involves material behavior, induced by irradiation, which is unique and not common in other areas of mechanical engineering. Besides, in research like this, modifications or customizations are often needed to address new problems or to explore new options in the fuel design optimization. The Finite Element Analysis Program (FEAP), an open-source research code developed by Taylor et al. [27], is chosen to perform this work because it is a reliable, multi-dimensional computer analysis system.
FEAP contains elements available to model multi-dimensional problems in linear or non-linear structural, solid mechanics and for linear heat conduction problems. Material models are provided in FEAP for elasticity, viscoelasticity, plasticity, and heat transfer constitutive equations [27]. The mesh can be generated by command line or imported from other codes. Both text and graphical output are available. In FEAP, users may add new routines for mesh generation, model element, new command language statements and new graphical display. A programmer’s manual is also available to facilitate modifications by users.

6.3.1 Modifications/additions to FEAP: user material models

As discussed before, the unique irradiation-induced material behaviors of PyC are not included as standard features in any FEM codes. To include these behaviors, modifications/additions to FEAP are needed. FEAP provides users access to add material models to elements by appending subprograms ‘umatinn’ and ‘umatln’ ($n = 0: 9$). The subprogram ‘umatinn’ reads in the parameters used by the model, and the subprogram ‘umatln’ is called by the element to calculate the stress at each Gaussian integration point [27]. In this work, user material models are developed to include both irradiation-induced shrinkage and creep strains in PyC.

The flow chart describing the addition of user material models to FEAP to include irradiation-induced shrinkage and creep is shown in Fig. 6.5. All the functions referred to in this chart are previously discussed in this chapter. A list of symbols is included to the right of the figure. Fig. 6.6 depicts the relationships among the new subroutines developed in this work and the main FEAP program. Most of the calculations are performed in ‘umat12.f’.

At each computation point (Gaussian point), if the material is PyC which is subject to shrink and creep under irradiation, the user material models developed here will be called. The radial and tangential shrinkage strain is calculated using the subroutine ‘shrink.f’. Given that the shrinkage data is only available at limited combinations of temperature and anisotropy, as shown in Fig. 6.2 and Fig. 6.3, linear interpolation is
1) read in parameters:
'thinp.f' written to read in $\nu_c$, $\Phi$, BAF, etc.; values for $E$, $\nu$, $\rho$, $T_0$, $T$, etc. obtained from common vector/variable $\vec{d}$, $x\vec{c}ur$, $td$ and $dt$; values for $\epsilon_t^{sw}$ and $\Phi$ obtained from history vector $\vec{h}n$; creep constant ($K$) and CTE ($\alpha$) calculated: $K = f_1(T, \rho) \ast kconst$; $\alpha = f_2(T) \ast aconst$.

2) calculate shrinkage strain $\epsilon_t^{sw}$:
'shrink.f' written to interpolate radial ($\epsilon_t^{sr}$) and tangential ($\epsilon_t^{st}$) shrinkage strain between temperature and BAF. $\epsilon_t^{sr}$ and $\epsilon_t^{st}$ calculated based on current $\Phi$, $T$, BAF.

3) convert $\epsilon_t^{sr}$ and $\epsilon_t^{st}$ into $\epsilon_t^{si}$:
current coordinates obtained by calling $\vec{x}cur$, unit radial vector $\vec{ur} = (\vec{r} - \vec{r}_0)/||\vec{r} - \vec{r}_0||$; two unit tangential vectors $\vec{ut}$ and $\vec{ut}'$, $\vec{ut}$ set as $(1,0,0)$ and $\vec{ut}' = \vec{ur} \times \vec{ut}$. $\epsilon_t^{sw} = f_3(\epsilon_t^{sr}, \epsilon_t^{st}, \vec{ur}, \vec{ut}, \vec{ut}')$.

4) calculate inelastic strain ($\epsilon_t^{ie}$):
$\epsilon_t^{ie} = \epsilon_t^{th} + \epsilon_t^{cr} + \epsilon_t^{sw}$; thermal strain $\epsilon_t^{th} = \alpha \ast td$, $\epsilon_t^{cr}$ and $\epsilon_t^{sw}$ calculated/obtained in previous steps.

5) calculate elastic strain ($\epsilon_t^{el}$) and stresses ($\sigma_i$):
material moduli $kk_{ij}$ obtained from common vector $\vec{d}$, and total strain $\epsilon_t^{tot}$ obtained from common vector $\vec{eps}$. elastic strain $\epsilon_t^{el} = \epsilon_t^{tot} - \epsilon_t^{ie}$; stresses $\sigma_i = kk_{ij} \epsilon_t^{el}$.

6) calculate creep stain at current time step ($\Delta \epsilon_t^{cr}$):
principal stresses $\sigma_{pi}$ converted from stresses $\sigma_i$ by calling 'eig3'; $\Delta \epsilon_t^{cr} = f_3(K, \nu_c, \Phi \ast dt, \sigma_{pi})$, then converted into $\Delta \epsilon_t^{cr}$ in Cartesian coordinate.

7) pass data into history vector ($\vec{h}n$):
$h_n(1:6) = h_n(1:6) + \Delta \epsilon_t^{ie}$, $h_n(7) = h_n(7) + \Phi \ast dt$.

List of Symbols:
$\nu_c$: creep Poisson’s ratio
$\Phi$: fast neutron flux
BAF: anisotropy factor
$E$: Elastic modulus
$\nu$: Poisson’s ratio
$\rho$: density
$T_0$: stress free temp.
$T$: temperature
$x\vec{c}ur$: current coord.
$td$: $T - T_0$
dt: time step
$\Phi$: fast neutron fluence
$K$: creep constant
$\alpha$: coeff. of thermal expansion
$kconst$: $K$ multiplier
$aconst$: $\alpha$ multiplier
$\epsilon_t^{cr}$: creep strain
$\epsilon_t^{sw}$: shrink strain
$\epsilon_t^{sr}$: radial shrink strain
$\epsilon_t^{st}$: tang. shrink strain
$\epsilon_t^{ie}$: inelastic strain
$\epsilon_t^{th}$: thermal strain
$\epsilon_t^{el}$: elastic strain
$\epsilon_t^{tot}$: total strain
$\sigma_i$: stress
$\sigma_{pi}$: principal stress
$\epsilon_t^{cr}$: prin. creep strain

Fig. 6.5: Flow chart describing the addition of user material models to FEAP to include irradiation-induced shrinkage and creep. All the functions referred to in this chart are previously discussed in this chapter. A list of symbols is included to the right of the figure.
'thinp.f': read user provided parameters from input.

The main FEAP program

'umatil2.f': call 'thinp.f' and common variables to read in parameters.

'eig3': convert stress to principal stress and return principal direction vector.

'shrink.f': calculate radial and tangential shrinkage strain.

'umatil2.f': calculate shrinkage, creep strain, stress and etc.

1) history vector \( \vec{h}_n \): store and retrieve creep strain and neutron fluence accumulated till last time step; 2) common vector \( \vec{x}_{cur} \): coordinate of current computation point; 3) common vector \( \vec{\epsilon}_{ps} \): total strain (determined by nodal displacement).

Fig. 6.6: Diagram of relationships among the new subroutines and the main FEAP program.
used to calculate shrinkage strain at actual values of temperature, anisotropy and flu-
ence. Once the radial and tangential shrinkage strains are calculated, it is required to
convert them into global strain by performing a coordinate transformation from local
radial and tangential directions to the global coordinate system (because the calcula-
tions in other part of FEAP is based on the global coordinate system). The details of
the conversion are shown in Step 3 in the flow chart in Fig. 6.5. For the creep strain,
since it is a function of principal stresses that keep changing over time, time integration
is needed. At each time step, the elastic strain is calculated using total strain and creep
strain accumulated till last time step (retrieved from history vector), as shown in Step
5 in Fig. 6.5. The stresses are then calculated and converted to principal stresses using
built-in subroutine ‘eig3’. The creep strain in principal directions now can be calculated
using principal stresses, creep constant, etc., as expressed in Eq. 6.2. Again the creep
strains in principal directions are converted into strains in global coordinate system (see
details in Step 6), and they are added to the creep strains induced in all previous time
steps and stored in history vector for use in the next time step. Creep constant mul-
tiplier \( (k_{\text{const}}) \) and thermal expansion coefficient multiplier \( (a_{\text{const}}) \) can also be read
in from the input file, which makes it convenient for one to study the impact of creep
or thermal expansion by artificially changing the creep constant or thermal expansion
coefficient.

Once this new user material model was added into FEAP, simple test cases, for which
results can be calculated by hand, were simulated and the results agreed with hand
calculations. Further tests for validations are also performed, and discussed in later
sections.

### 6.3.2 Modifications to FEAP: time-dependent thermal boundary conditions

During transient conditions such as reactor startup, shutdown, power surge, loss of
coolant, etc., the thermal condition keeps changing due to transient thermal boundary
conditions. Modifications are needed for FEAP to handle time-dependent thermal
boundary conditions. The easiest way to add this new capability is to modify existing subroutines. FEAP has a ‘convection element’ that can be used with thermal elements to impose boundary thermal flux. This boundary condition is expressed as below:

$$q_n = q_0 + h(T^n - T_f^n),$$

(6.5)

where $q_n$ is total boundary thermal flux; $q_0$ is a constant prescribed flux; $h$ is a surface parameter (e.g., convective heat transfer coefficient); $n$ is an integer exponent for convection/radiation and $T_f$ is free-stream temperature. Setting $n = 1$ gives a linear convection condition whereas setting $n = 4$ gives the Stefan-Boltzman radiation approximation [27].

With minor modifications, this ‘convection element’ can be upgraded to handle time-dependent boundary condition. The new boundary condition is expressed as below:

$$q_n(t) = q_0 \ast g_1(t) + h \ast g_2(t) \ast \left[ (T(t))^n - (T_f \ast g_3(t))^n \right],$$

(6.6)

where $g_i(t)$ ($i = 1 : 3$) are functions of time that can be defined by user in the input file. Extra steps are taken to read these time functions in FEAP and to ensure that these modifications are compatible with the main FEAP program. No extra effort is needed to modify FEAP to allow these time dependent functions because FEAP already has a built-in feature—“proportional loading”, which implements time-dependent pressure or nodal forces etc. The time dependent function can be of various forms. An easy way is to input the function in tabular format (a series of discrete data sets). The data between the discrete points is linearly interpolated.

6.3.3 Stress model geometry setup

As discussed before, it is deemed sufficient to include only the outer three coating layers of the TRISO particle, because the buffer layer is made of porous carbon. The effects of the kernel and the buffer layer are accounted for by imposing thermal and pressure boundary conditions on the inner surface of the IPyC layer. Model is further
simplified by assuming that the TRISO particle is in an axisymmetric state about Y axis. Note that asymmetric conditions can still be modelled in this axisymmetric model by applying different boundary conditions etc. at different polar angles. Given the purpose of this work, to include all major physics into the stress model and to evaluate the impacts of different material properties and boundary conditions on the stress state, this axisymmetric model is adequate to account for most of the 3D effects and has the benefit of dramatically lower time and computation costs than a full 3D model. Note that the modified FEAP has full 3D capability.

FEAP does not have a graphical interface for mesh generation, and command lines are used to generate mesh. A simple way to generate a mesh is to define each of the nodal point by its coordinate and then connect them to form elements. More advanced ways, such as those using the utilities like “block”, to build a mesh are provided in FEAP. Each of the 3 layers can be built using a block of quadrilateral elements. The geometry is shown in Fig. 6.7. Both the IPyC and OPyC layers use the same material—PyC, and thus they are indicated by the same color (magenta). The SiC layer is colored in yellow. This 2D mesh uses axisymmetric element (over $0 < \phi < \pi$) to account for the 3D effect, so it is actually a 3D spherical shell of 3 layers. Note that the number of elements in this figure is reduced for clarity. In the model used to conduct the analysis, for each coating layer, there are 10 layers of elements in the radial direction and 100 layers in the tangential direction. The mesh is considered sufficiently refined because models with twice as many elements give similar results (less than 1% difference) as this one.

6.3.4 Boundary conditions

Different boundary conditions are applied in the stress model shown in Fig. 6.7. On the outer surface of the OPyC layer, pressure of 6 MPa is applied uniformly to simulate the coolant pressure. (Although coolant does not directly contact a TRISO particle, the coolant pressure is transmitted through the pebble structure onto each TRISO particle in it.) The temperature on the outer surface is fixed in a static model, and time-dependent
Fig. 6.7: Simplified mesh of the TRISO stress model. Both the IPyC and OPyC layers use the same material–PyC, and thus they are indicated by the same color (magenta). The SiC layer is colored in yellow. Note that the number of elements in this figure is reduced for clarity. The arrows represent inner and outer pressure.

in a transient model. As discussed in Chapter 2, the temperature on the particle outer surface depends on the relative position of the TRISO particle in the pebble, and on the thermal condition of the pebble itself.

On the inner surface of the IPyC layer, time-dependent pressure is applied, which is caused by the buildup of fission gases. As discussed in the previous chapter, the high-end gas pressure is 24.6 MPa at burnup of 72.78 GWd/tU. In the stress analysis in this chapter, the maximum fast neutron fluence is $3 \times 10^{25} \text{ n/m}^2$, which corresponds to a maximum burnup of 41.4 GWd/tU (or irradiation time of 835 days). So, the corresponding high-end gas pressure (after multiplying a safety factor of 1.12 to obtain conservative results of stresses) in this case is 15.75 MPa. The pressure is assumed to increase linearly as a function of time and it is implemented using the “proportional loading” feature. Since this model uses axisymmetric elements, each of them, as shown in Fig. 6.7, represents a full ring of elements. The pressure loading on each axisymmetric element is proportional to the length of ring it represents. Since it is tedious to apply different pressure loadings on each element, FEAP has a feature called “pressure element” that takes a specified uniform pressure and transforms it to axisymmetric...
loading accordingly. As for the thermal condition, most of the heat is produced in the kernel and some of it is produced in the buffer layer. Hence, thermal flux is applied at the inner surface of IPyC. The thermal flux integrated over the inner surface equals to the total heat produced in the kernel and buffer layer (total power per TRISO particle is assumed to be 24.6 mW). The thermal flux is set as constant in a static model and time-dependent in a transient model. Details of how to set time-dependent thermal flux are discussed in subsection 6.3.2.

As shown in Fig. 6.7, the horizontal movement of the nodes with \( X = 0 \) is restrained because the model is assumed axisymmetric around the Y-axis. The vertical movement of one node (can be any node) is also restrained to prevent rigid-body motion.

### 6.4 Stress results of a TRISO particle

The stress model of a TRISO particle is tested with various material properties, different thermo-mechanical conditions, various partial defects, etc. The results are presented and discussed below. First, a stress model is developed to compare results with those obtained from Miller’s model [13].

#### 6.4.1 Comparison with Miller’s model, impacts of shrinkage, creep, \( \nu_{c} \), and particle size

Miller et al. [13] developed a stress model of a TRISO particle using Abaqus which included all the major physics affecting the stress state. In order to benchmark our codes (FEAP with the modifications introduced in this work), a stress model using the same parameters is set up to compare with Miller’s results. In this model the stresses in the particle are calculated over the irradiation time. The fast neutron fluence increases from 0 to \( 3 \times 10^{25} \) n/m² from the beginning to the end (\( t = 1.2 \times 10^{7} \) sec.). The problem geometry is shown in Fig. 6.7. The overall diameter is 631 \( \mu \)m, and the thickness of IPyC, SiC and OPyC are 40, 35 and 43 \( \mu \)m respectively. The outer pressure is 6.4 MPa and the internal pressure increases from 0 to 23.7 MPa over time. The temperature is
Fig. 6.8: Time history of tangential stresses in IPyC and SiC: (a) calculated with Miller’s model using Abaqus (the fast neutron fluence is $3 \times 10^{25}$ n/m$^2$ when the time is $1.2 \times 10^7$ sec.) [13]; (b) calculated in this work using modified FEAP.

assumed to be 1200°C uniformly; the BAF is assumed to be 1.16; the creep Poisson’s ratio ($\nu_c$) is assumed to be 0.5. The CEGA creep constant (see Table 6.2) is used. One hundred time steps are used to simulate the fast neutron fluence increasing from 0 to $3 \times 10^{25}$ n/m$^2$ (100 time steps are determined to be sufficient since no improvement is observed if 200 time steps are used).

The time history of tangential stresses in IPyC and SiC in Miller’s model and in this model are displayed in Fig. 6.8. Note that both plots are on the same time frame because the fuel has the same exposure of fast neutron fluence. As shown, the results are very close, demonstrating that the modified FEAP code works well. The tangential stresses in IPyC and SiC are tensile and compressive, respectively, because both IPyC and OPyC shrink under irradiation and exert compression on the SiC layer; while on the other hand SiC is more rigid and hinders the shrinkage of PyC, keeping the PyC layers in tension as a result. Contrary to conventional wisdom, the tangential stresses do not increase continuously with time as a result of ever-increasing internal gas pressure; the stresses peak at about one third of the irradiation time. After that creep in PyC layers relieves stresses in both layers, counteracting the increase of PyC shrinkage and internal gas pressure.
Fig. 6.9 shows radial and tangential stresses in the IPyC, SiC and OPyC layer. As shown, tangential stresses in the IPyC and SiC layer are the two largest stresses. Note that the stresses are taken from the middle element in each layer. The tangential stress in OPyC is \(\sim 40\%\) lower than that in IPyC. Because these two layers are made of the same material, OPyC is less important for evaluation of failure rate. Hence, the tangential stresses in IPyC and SiC are the main focus for failure evaluation.

Test models are also developed to evaluate the separate effects from internal gas pressure, PyC shrinkage, and PyC creep on particle’s stress state. The first model includes only pressure (no shrinkage or creep); the second model adds shrinkage to the first one (no creep); the third model (referred to as “base case”) includes all three (also shown in Fig. 6.8(b)). The results are shown in Fig. 6.10. The stress results of the first model is shown in Fig. 6.10(a). As shown, IPyC is under slight compression, and the tangential stress in the SiC layer changes from compressive to tensile because of the increasing internal pressure. Comparing with the base case (see Fig. 6.8(b)), the magnitude of maximum tangential stress in SiC of this pressure-only model is only \(\sim 1/30\)th of that in the base case, indicating that gas pressure plays only a minimal role in the overall
stress state. This pressure-only model is very similar to the conventional pressure vessel model, and the results of this model also indicate that the failure probability of both IPyC and SiC is minimal because the stresses are low and the IPyC layer is always under compression (thus less likely to fail), which is contrary to the observation of macro cracks in IPyC layer in irradiation experiments [13, 17].

The comparison between the second model (that includes everything but creep) and the base case is shown in Fig. 6.10(b). As can be seen, the shrinkage of PyC is the major contributor to the stresses. Without the relaxation mechanism introduced by creep, the stresses will continuously grow and the magnitude of stresses are so high that both IPyC and SiC will certainly fail. The results of this model emphasize that both shrinkage and creep of PyC play a major role in the stress state of the TRISO particle.

Another test model is developed to evaluate the impact of creep Poisson’s ratio ($\nu_c$), and the results are shown in Fig. 6.11. As shown, $\nu_c$ makes a nontrivial impact and the stresses are smaller for the $\nu_c = 0.4$ case, which is consistent with the creep strain equation (Eq. 6.2). According to this equation, lower $\nu_c$ gives higher effective stress and then higher creep strain, and thus results in lower stresses.

In this work, a larger-sized TRISO particle is used than in Miller’s model: the dimensions are shown in Table 2.3 and the outer diameter (OD) is 920 µm (the OD in Miller’s model is 621 µm). A model using the larger particle size (with slightly different thickness of the three outer coating layers) is developed to evaluate the impact of particle size, while all other parameters (including pressure etc.) remain the same. The results are shown in Fig. 6.12. As shown, the peak stresses are lower in the larger-sized particle ($\sim15\%$ lower in SiC and $\sim25\%$ lower in IPyC).

6.4.2 The impacts of irradiation temperature, power, CTE, gas pressure, BAF, and layer thickness

From this point forward, a creep constant that is twice as large as the value determined by the CEGA relation (as shown in Eq. 6.3 and Eq. 6.4), coupled with a creep Pois-
Fig. 6.10: Time history of tangential stresses in IPyC and SiC: (a) the model includes pressure only; (b) the model includes pressure and shrinkage but no creep vs. the base case.
Fig. 6.11: Comparison of tangential stresses in IPyC and SiC when two different creep Poisson’s ratios are used ($\nu_c = 0.4$ vs. $\nu_c = 0.5$).

Fig. 6.12: Comparison of tangential stresses in IPyC and SiC between a larger particle ($OD = 920 \mu m$) and a smaller one ($OD = 621 \mu m$) ($T = 1200^\circ C$).
son’s ratio of 0.4, are used. (Because Miller et al. reported that models using the larger creep constant better match experiments [17, 70].) The mesh is also based on the larger-sized TRISO particle ($OD = 920 \mu m$). The external pressure is 6 MPa, and the internal pressure is 15.75 MPa at the end (at the maximum neutron fluence of $3 \times 10^{25} \text{n/m}^2$) based on the calculations and assumptions in Chapter 5. In this subsection, the impacts of irradiation temperature, creep constant, power, CTE and layer thickness on the stresses are evaluated and discussed.

Under different irradiation temperature, PyC shrinks and creeps differently; the thermal expansion is different as well but its impact is minimal under normal condition (will be discussed later). Fig. 6.13 shows how creep constant and shrinkage strain change with irradiation temperature derived from Eq. 6.4 and Fig. 6.2(a) respectively. To enable direct comparison, all values are normalized to the corresponding value at 700°C. The shrinkage strain is shown under two different neutron fluence ($1.5$ and $3.0 \times 10^{25} \text{n/m}^2$). Note that creep strain can not be obtained without integration over time and knowing the stresses, thus only creep constant is shown here. As shown, irradiation temperature has a larger impact on creep constant.

To further study the impact of irradiation temperature on stress states, models are developed to calculate the stresses under three different temperatures (700, 1000 and 1200°C). Fig. 6.14 shows the time history of the tangential stresses in IPyC and SiC for the three temperatures. Comparing the 1200°C case in this figure with the 920 μm OD case in Fig. 6.12, both cases are the same except that this case uses twice larger creep constant. The increased relaxation caused by the amplified creep constant reduces the peak stresses approximately by a factor of two. As shown in this figure, higher stresses are observed at lower irradiation temperature, which is consistent with earlier discussions: lower temperature reduces both creep and shrinkage but has a larger impact on creep. The implications of these results are that the pebbles situated near the coolant inlet have a higher percentage of failed TRISO particles than the ones near the outlet.

Another set of models are developed to evaluate the impact of thermal power, coefficient of thermal expansion (CTE), internal gas pressure, and anisotropy (BAF) on
Fig. 6.13: Variation of creep constant and shrinkage strain with irradiation temperature.

Fig. 6.14: Tangential stresses in IPyC and SiC under three different temperature (700, 1000 and 1200°C respectively).
stress states. Fig. 6.15 shows the results obtained in this numerical experiment. Higher thermal power leads to higher temperature gradients across the three coating layers. However, the thermal conductivity of these three layers are relatively high and the dimensions are small, thus the overall temperature change across the three layers is small (less than 1°C as shown in Fig. 2.16). CTE affects the thermal strain as well. However, since the temperature gradient is small, the impact is minimal, as seen in Fig. 6.15(b). To simulate situation depicting higher gas release fraction or higher fuel burnup, the internal gas pressure is assumed to be twice as large, but as discussed earlier since the stress states are dominated by creep and shrinkage, the difference in stress due to higher gas pressure is expected to be small. As shown in Fig. 6.15(a) and (b), no significant difference is observed due to different power, CTE or internal pressure. Lastly, higher shrinkage strain is observed in PyC with higher anisotropy (see Fig. 6.3), and thus higher stresses are expected, as seen in Fig. 6.15(c).

The effects of different thicknesses of IPyC, SiC and OPyC layers are also studied. Three different cases are developed and in each case one of the three layers is made 30% thicker. Fig. 6.16 shows the results, compared with the base case. The variation of the layer thickness has minimal impact on the tangential stress in IPyC, but has nontrivial impact on the stress in SiC. Larger SiC thickness helps reduce stress in SiC, whereas larger IPyC or OPyC thickness increases stress in SiC because of the larger integral load caused by the PyC shrinkage in thicker IPyC or OPyC layers.

6.4.3 Stress under transient conditions

With the modifications to the FEAP code, thermo-mechanical transient conditions can also be simulated. In this part, two different transient conditions are modeled. Case 1: the thermal power of the particle is assumed to be doubled in 100 seconds. Case 2: it is assumed that the pebble is taken outside of the reactor at the end of fuel life and is then left to cool down. The transient processes start at the fluence around $3 \times 10^{25}$ n/m$^2$ in both cases. In Case 1, based on the thermal model for a pebble as described in Chapter 2, the temperature in the TRISO at the mid radius of the pebble is increased by
Fig. 6.15: Tangential stresses in IPyC and SiC: (a) with twice the thermal power or twice the internal gas pressure; (b) for two different values of CTE (T=700°C) (note that stress free temperature (T₀) is 1200°C); (c) for two different BAFs (1.08 and 1.16).
Fig. 6.16: Tangential stresses in IPyC and SiC for three different cases (in each case one of the three coating layers is made 30% thicker).

90°C due to the increased power (assuming the coolant temperature does not increase). The creep and the shrinkage strains during these 100 seconds do not change, because the additional irradiation over such a short period is insignificant and such irradiation-induced changes take place at much larger time scales. The thermal strain changes significantly due to the temperature change. Fig. 6.17(a) shows stress results of Case 1. As expected, during the transient process the thermal strain is reduced due to the rising temperature ($T_0 = 1200^\circ$C), thus resulting in smaller stresses. Since thermal strain accounts for only a small fraction of the total strain (dominated by shrinkage and creep), the impact of this power transient is not significant. Fig. 6.17(b) shows the stress results for Case 2. After being taken out of the reactor core, the TRISO temperature is assumed to decrease from 1000 to 100°C in 4 hours. The ambient pressure decreases from 6 MPa to 0.1 MPa at $t = 0$. The creep and shrinkage strains remain unchanged since no extra significant irradiation is introduced during this transient process. As shown, there is a sudden change at the beginning of the transient process due to the abrupt loss of ambient pressure. The stresses increases slowly due to the decreasing...
Fig. 6.17: Time history of tangential stresses in IPyC and SiC: (a) Case 1, the power surges 100% in 100 seconds; (b) Case 2, the TRISO particle (along the pebble) is taken outside of reactor core and is left to cool down. Note that the transient conditions in both cases start \((t = 0)\) at the fluence around \(3 \times 10^{25}\) n/m\(^2\). After that the range 3–6 on the X-axis represents the entire transient time for the convenience of illustration, and 6 on X-axis corresponds to \(t = 100\) seconds in Case 1 and 4 hours in Case 2, respectively.

temperature (lower temperature means higher thermal strain because the stress free temperature is as high as \(1200\)°C).

6.4.4 Stress in a defective TRISO particle

Defects can be produced during the manufacturing process of TRISO particles, especially when the particles cool down from the high manufacturing temperature (higher than \(1200\)°C) to room temperature, when thermal stresses can introduce cracks in the IPyC or OPyC layer. Cracks in IPyC or debonding between IPyC and SiC are likely to occur under normal operation, when IPyC is always under tension and the tangential stress reaches above 100 MPa (as shown in the previous sections). Palladium, a fission product, is known to react with SiC and form weaker compound. In this part, several models are developed with different defects: Case 1 assumes there is a crack in IPyC all through its thickness; Case 2 assumes IPyC debonds from SiC in the region \(\theta = -30\) to 30°; Case 3 assumes that SiC is *corroded* by Pd (resulting in Young’s modulus being
reduced by a factor of two) in an area spanning 60\% of the SiC layer thickness, from $\theta = -30$ to $30^\circ$.

Fig. 6.18 shows the stress results for Case 1. Fig. 6.18(a) shows the crack in IPyC after the irradiation when the crack has opened up due to the tensile stresses. Since this is an axisymmetric model, the crack represents a ring of crack. Fig. 6.18(b) shows tangential stresses around the crack at the fast neutron fluence around $3 \times 10^{25}$ n/m$^2$. Fig. 6.18(c) shows the tangential stresses in a few elements in IPyC or SiC. Note that “mid” means the middle element in a particular layer; “tip” means the element at the crack tip. As shown in this figure, stresses in all other elements, except the “tip of SiC” element, are relaxed because of the crack, whereas the tangential stress in the SiC element right at the IPyC crack tip becomes tensile (it is compressive in an intact TRISO particle.), and it reaches its first local maximum around fluence of 1.0, drops for a while and continues to grow after that. The growth at later time is caused by three factors: 1) the growth of the internal pressure; 2) the increase of shrinkage strain at higher fluence; 3) the acceleration in tangential strain after fluence of 4.0, as shown in Fig. 6.2(b). Since in an intact particle, SiC as a whole is always under compression as shown in previous figures, the failure probability of SiC in this defective particle dramatically increases due to the tensile stress in the “tip” element and the probability increases at higher fluence (or burnup).

Fig. 6.19 shows the results for Case 2. Fig. 6.19(a) shows the debonding at the interface between IPyC and SiC (indicated by the yellow line). Fig. 6.19(b) shows the tangential stresses in a few elements in IPyC or SiC in the debonding case. Note that “tip of SiC” in this case means the element in SiC right next to the debonding interface. Compared to a normal particle, there are no significant changes in stresses except that the tangential stress in the “tip” SiC element increases by $\sim 30\%$ due to the loss of support from IPyC.

Fig. 6.20 shows results for Case 3. Fig. 6.20(a) shows the corroded area in SiC (by Pd attack) which covers from $\theta = -30$ to $30^\circ$ through 60\% of SiC thickness, and Young’s modulus in this area is assumed half that of SiC. Fig. 6.20(b) shows the tangential stresses in a few elements in IPyC or SiC. Note that “mid corroded SiC” means the
Fig. 6.18: (a) The crack in IPyC after the last time step (number of elements reduced for clarity); (b) tangential stresses around the crack at the fast neutron fluence around $3 \times 10^{25} \text{ n/m}^2$; (c) time history of tangential stresses in a few elements in IPyC or SiC in the cracked-IPyC case. Note that “mid” means the middle element in a particular layer; “tip” means the element at the crack tip.
Fig. 6.19: (a) The debonding at the interface between IPyC and SiC (number of elements reduced for clarity); (b) time history of tangential stresses in a few elements in IPyC or SiC in the debonding case. Note that “mid” means the middle element in a particular layer; “tip of SiC” means the element in SiC right next to the debonding surface.

There are no significant changes in stresses in most elements compared to an intact particle except that the tangential stress in the “mid intact SiC” element increases by $\sim 33\%$ as a result of the corrosion.

### 6.5 Failure prediction of TRISO particles

Both Pyrocarbon and SiC are generally considered as brittle materials, and their failure probability are expected to follow the Weibull statistical theory [71]. The failure probability of a particular layer can be calculated as follows [66, 72]:

$$f(t) = 1 - \exp \left( -\ln 2 \left( \frac{\sigma(t)}{\sigma_m} \right)^m \right), \quad (6.7)$$

where $\sigma_m$ is the Weibull mean fracture strength, and $m$ is the Weibull modulus. The values of these two parameters are scattered significantly in literature, and the rec-
Fig. 6.20: (a) The corroded area in SiC, from -30 to 30° through 60% of SiC thickness (Young’s modulus reduced by half in this area); (b) time history of tangential stresses in a few elements in IPyC or SiC in the corrosion case. Note that “mid” means the middle element in a particular layer; “mid corroded SiC” means at the middle of corroded part of SiC, “mid intact SiC” means middle of uncorroded part of SiC.

Recommended values in the CEGA report are adopted in this work because that report reviewed a variety of data reported in literature [15]. Table 6.3 shows the Weibull mean fracture strength ($\sigma_m$) and the Weibull modulus ($m$) in PyC and SiC used in this work [15, 17]. Failure probability in IPyC and SiC are discussed below. Since stresses in OPyC are always smaller than in IPyC (see Fig. 6.9), failure in OPyC is not discussed.

<table>
<thead>
<tr>
<th>Material</th>
<th>Strength ($\sigma_m$, MPa)</th>
<th>Weibull modulus ($m$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PyC</td>
<td>300</td>
<td>9.5</td>
</tr>
<tr>
<td>SiC</td>
<td>500</td>
<td>6.0</td>
</tr>
</tbody>
</table>

Table 6.3: The Weibull mean fracture strength ($\sigma_m$) and the Weibull modulus ($m$) in PyC and SiC [15, 17].
6.5.1 Failure probability in IPyC

Based on Eq. 6.7, along with the stresses presented previously in this chapter, the failure probability of IPyC in each previous case can be calculated. Since one of the purpose of this study is to evaluate the impacts of different variables (such as material properties, design parameters, or external conditions) on failure, the comparison of failure probability of IPyC for selected cases are summarized in Table 6.4. As shown, lower \( \nu_c \) or BAF help reduce IPyC failure, whereas lower irradiation temperature or overall diameter increases IPyC failure. The design requirement of TRISO particle failure is usually of the order of 1E-4. The reason why the failure in Case A and B is unreasonably high is because these two cases use the standard CEGA creep constant, which underestimates the creep and thus overestimate the stresses. In most part of this work, a creep constant equal to twice the CEGA value is used (as in Case C and D), and the failure predictions of IPyC in these cases generally agree with the findings by Miller et al. [13, 17], and lie near the borders of the design requirement except for the case with low irradiation temperature (\( T = 700^\circ C \)). Note that when IPyC fails, the particle is not considered failed until SiC fails as well.

<table>
<thead>
<tr>
<th>Case</th>
<th>Figure ID</th>
<th>variables</th>
<th>stress (MPa)</th>
<th>failure prob.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Fig. 6.11</td>
<td>( \nu_c = 0.4 )</td>
<td>245</td>
<td>9.63E-2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \nu_c = 0.5 )</td>
<td>335</td>
<td>8.62E-1</td>
</tr>
<tr>
<td></td>
<td>Fig. 6.12</td>
<td>( OD = 621 )</td>
<td>340</td>
<td>8.97E-1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( OD = 920 )</td>
<td>270</td>
<td>2.25E-1</td>
</tr>
<tr>
<td></td>
<td>Fig. 6.14</td>
<td>( T = 700 )</td>
<td>220</td>
<td>3.58E-2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( T = 1000 )</td>
<td>120</td>
<td>1.15E-4</td>
</tr>
<tr>
<td></td>
<td>Fig. 6.15(c)</td>
<td>( BAF = 1.08 )</td>
<td>100</td>
<td>2.03E-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( BAF = 1.16 )</td>
<td>130</td>
<td>2.46E-4</td>
</tr>
</tbody>
</table>

Table 6.4: Comparison of the failure probability of IPyC for different variables. Note that \( \nu_c \) is creep Poisson’s ratio; “OD” is overall TRISO particle diameter (\( \mu m \)); “T” is irradiation temperature (°C); and BAF is anisotropy factor.
6.5.2 Failure probability in SiC

In general, compressive stresses are not considered to contribute to failure, but when the stress magnitude are high, failure will be caused by compression. Unfortunately at this point, no experimental data available in literature to predict failure of SiC under compression. The SiC layer, under most circumstances, is always under compression as shown previously. As discussed before, the magnitude of compressive stresses in part of SiC are increased in several cases such as lower irradiation temperature, higher BAF, lower SiC thickness, debonding and corrosion to SiC. The change of failure probability of SiC however can not be estimated in such scenarios until a mechanism becomes available to predict failure caused by compressive stresses.

One exception is that when there is a through-thickness crack in IPyC, leading to stress in some parts of SiC becoming tensile (see Fig. 6.18(c)). In this “cracked” IPyC case, the failure probabilities of SiC are 2.84E-3 at low burnup and 4.65E-2 at high burnup, which are much higher than the design requirement (in the order of 1E-4). This finding indicate that once IPyC fails by radial cracking, SiC is likely to follow and thus cause the whole particle to fail. So it is important to prevent radial cracks from occurring in IPyC.

6.6 Summary

In this chapter, 3D axisymmetric stress models are developed using FEAP. Modifications are made to FEAP to include PyC shrinkage and creep etc. The modified code is benchmarked against Miller’s results and good agreement is observed. A few variables are studied to evaluate their impacts on stresses and failure probabilities. These variables include creep constant, creep Poisson’s ratio, particle size, irradiation temperature, power, CTE, internal gas pressure, BAF and layer thickness. Some thermal transient conditions and defective cases such as crack in IPyC, debonding, and corrosion to SiC are also studied. Among all, a few variables/conditions have significant impacts on stresses and failure probabilities, namely: shrinkage strain, creep constant,
creep Poisson’s ratio, particle size, irradiation temperature, BAF and crack in IPyC. Order of magnitude of stresses resulting from temperature changes, pressure buildup due to gas generation, and due to PyC shrinkage/creep show that in the case of TRISO particle (when using specific empirical constants or existing dataset found in literature to calculate shrinkage/creep strains), stresses due to temperature changes and internal gas pressure are orders of magnitude lower than those resulting from shrinkage/creep. Given the scatter/uncertainty in data regarding irradiation-induced shrinkage and creep strain in PyC, future validations are needed.
7 CONCLUSIONS AND FUTURE WORK

7.1 Summary and conclusions

Pebble-bed and prismatic reactors are two competing designs for the High Temperature Gas Reactor (HTGR), widely recognized as one of the top candidates for the Next Generation Nuclear Power-plant (NGNP) fleet. TRISO particles are a key component of the HTGR core design, and the success of the reactor depends on the safety and quality of the TRISO particles. During operation, a TRISO particle undergoes complex thermo-mechanical processes. Fission gases accumulate inside the kernel and the buffer layer, and lead to buildup of internal pressure. Uneven thermal conditions lead to asymmetric thermal expansion. The pyrolytic carbon, in both the IPyC and OPyC layers, is known to experience dimensional change (shrinkage or swelling) under fast neutron irradiation. In the mean time, both the IPyC and OPyC layers creep as a function of stress and fast neutron fluence. Macro cracks in the IPyC layer, corrosion in the SiC layer due to chemical attack, and debonding at the interface between IPyC and SiC have been observed in post-irradiation examination. All of these processes further complicate the stress states in a particle and might lead to failure of a single coating layer or the particle as a whole.

In this work, a comprehensive, multi-dimensional and multi-physics computer model was developed to simulate and evaluate TRISO fuel performance. This comprehensive computer model makes use of existing nuclear and mechanical codes (with modifications introduced as part of this work), and also the codes developed in this work to simulate all the main processes taking place in a TRISO particle. Below are a list of the main accomplishments of this work:

- **3D heat transfer model:** A 3D thermal model is developed using finite dif-
ference method. The temperature calculated using this model is compared to analytical solutions and to the results reported in literature. Good agreements are observed. Since TRISO particles are embedded inside pebbles, two thermal models are developed: one for the pebble and the other for the TRISO particle. The pebble model provides boundary conditions for the particle model. Temperature in a pebble is calculated at different power levels and under various convective boundary conditions. The neighboring pebbles may block the coolant flow around a pebble and may cause hot spots. The impact of such blockages was quantified using this thermal model. The temperature inside a TRISO was calculated under different conditions. The increase of temperature caused by a gas bubble (with lower thermal conductivity) inside the kernel was quantified as well. The thermal condition has to be monitored closely to ensure the safety of the fuel. The thermal gradient is also one of the main factors that dictate some other processes. The thermal model developed in this work is a useful tool to quantify the thermal condition in a pebble and a TRISO particle under various conditions.

• **3D neutronics model:** A 3D neutronics model is developed using MCNP5/X. Unit-cell model is used to represent the random packing of TRISO particles inside a pebble, and also of pebbles inside a reactor core. The neutron energy spectrum, fast neutron fluence, heat generation rate inside a particle and a pebble are quantified. Burnup calculations are also performed by coupling this model with CINDER to track the changes of a few important isotopes such as Xe, Kr, Ag, etc. Modification is also made to the data library to enable CINDER to track helium production caused by ternary fission. The mass and composition of gaseous elements, and some other key elements such as silver, palladium, cesium, etc., produced in the fuel are quantified. The sensitivity of gas production in different fuel configurations and enrichments are also quantified. (The ratios between some gaseous isotopes (e.g., $^{136}$Xe vs. $^{86}$Kr) can be used as a signature of for the fuel content inside a reactor, which might find applications in nuclear
safeguard.) In short, the results obtained using this neutronics (including burnup) model provide valuable dataset for the overall performance model, and also for researchers in other areas of nuclear engineering.

- **Gas release model:** The fractional gas release on both intra- and inter-granular level are calculated using White and Tucker’s model. The gas pressure inside the buffer layer is also quantified.

- **3D stress model:** The open-source finite element code FEAP is chosen for the stress analysis in this work. Modifications are made to FEAP to include PyC shrinkage and creep, and also to model time-dependent thermal boundary conditions. The modified code is benchmarked with Miller’s results that are obtained through the commercial code Abaqus, and good agreement is observed. Axisymmetric stress model is used to account for the 3D effect while reducing the computation costs. A few variables are studied to evaluate their impacts on stresses and failure probabilities. These variables include creep constant, creep Poisson’s ratio, irradiation temperature, BAF, layer thickness, etc. Some transient thermal conditions and defective cases, such as a radial crack in IPyC, debonding and corrosion to SiC, are also studied. Among all, a few variables/conditions have significant impacts on stresses and failure probabilities, and they are: shrinkage strain, creep constant, creep Poisson’s ratio, particle size, irradiation temperature, BAF and crack in IPyC. Order of magnitude of stresses resulting from temperature changes, pressure buildup due to gas generation, and due to PyC shrinkage/creep show that in the case of TRISO particle (when using specific empirical constants or existing dataset found in literature to calculate shrinkage/creep strains), stresses due to temperature changes and internal gas pressure are orders of magnitude lower than those resulting from shrinkage/creep. Failure probabilities of both IPyC and SiC are also calculated. The failure probability of IPyC under most conditions borderlines with the design requirement (1E-4) except under low irradiation temperature. The failure probability of SiC under normal conditions is minimal because it is always under compression mainly caused by
PyC shrinkage; except when there is a radial crack in IPyC, in which case the stress in part of SiC becomes tensile and the failure probability is higher than 1E-4, and increases at higher burnup.

The comprehensive fuel performance model developed in this work is a useful tool to quantify and evaluate the thermal, nuclear and mechanical conditions in the TRISO fuel. Some of the results obtained in this work might find applications in other areas. Some of the codes or modifications to existing code developed in this work can easily be adapted for fuel performance modeling of other forms of nuclear fuel.

7.2 Suggested future work

This thesis work obviously can not model everything relevant to fuel performance of TRISO fuel. A few items are suggested for future work:

- **Automated system to connect various parts of this model:** Currently the various parts of this performance model are manually linked with one another. A computer automated system with better visualization is desired, e.g., a platform in which one would see visualized change in stress immediately after the change of thermal conductivity. Some modifications to FEAP are also desired to enable it to produce customized graphical outputs.

- **Further validation of PyC shrinkage and creep data:** It is found in this work that the irradiation-induced shrinkage and creep of PyC have a dominant impact on the stress state and thus failure. Given the significant scatter/uncertainty in the data reported in literature, future validations are needed and conclusive correlations are also desired to predict PyC shrinkage and creep based on some combination of the PyC attributes/conditions.

- **Shuffling of pebbles in the reactor:** Currently the pebbles inside the core are assumed stationary. In reality, a pebble shuffles around in the core and it is also taken in and out of the core during refueling, thus usually getting exposed to
different thermal and nuclear conditions during its lifetime. A model is needed to track the movement of the pebble and to study the impact of the movement.

- **Prediction of failure of SiC under compression:** At this point, there is no experimental data to support the failure prediction of SiC under compressive stresses. (There might be some mechanism to predict failure of some brittle material, similar to SiC, under compression though.) Since in a TRISO particle, the SiC layer is always under compression in most conditions. The compressive stresses in SiC are so high that an evaluation of failure caused by the compression is desired. Experimental data is needed to enable such evaluations.

- **Full 3D stress models:** Due to the time limit, only 3D axisymmetric stress models are tested. Full 3D models are needed to be simulated. Note that the modifications introduced in this work to FEAP have full 3D capabilities. The main difficulties lie in generating the full 3D mesh and the extra computer time it takes to solve the full 3D stress model. Improvements of the mesh generation capability of FEAP are also desired.

- **Coupling the coolant field with the thermal model:** Currently the coolant flow around the pebbles is simplified. Fluid flow models are needed to simulate the coolant flow in the core on static and transient conditions. Coupled with the thermal model developed in this work, this model would enable accurate temperature prediction under accident scenarios such as loss of coolant. By coupling with the neutronics model, temperature feedback on heat generation induced by the accident are also possible.
REFERENCES


Jianwei Hu was born in a remote village of You County, Hunan province of China in 1978. His parents are both peasants working on several pieces of small rice fields. The working environments were harsh during the hot and humid summer (the busiest season for rice growers) and the labor was intense without help of any powered tools or transportation mechanism. His parents worked hard and harvested barely enough to support the family. His parents also raised pigs, chickens and ducks to obtain additional income. Starting as a small child, Jianwei worked on the rice fields along with his parents, and learned the value of hard work.

Jianwei was always the top 2 students in his class and his year through elementary school and middle school. Jianwei considered himself lucky to be admitted to a “experimental class” in the middle school, after which he considered seriously to join a technician school because his family were afraid that they might not be able to support him through high school or college. A rare opportunity showed up: a key high school of Hunan province opened door for the first time for top talents of You County. Jianwei did well in the entrance exams and was very luckily admitted to the only “Olympic class” of the school among 30,000 competitors.

Jianwei received his B.E. in Nuclear Engineering from Xi’an Jiaotong University (China) in July 1997.

During his studies for the B.E. degree, Jianwei completed the graduation project of forced and natural heat transfer of a research reactor. He has studied general engineering courses such as heat transfer, material mechanics, fluid mechanics, machine manufacture, cartography, etc. He also studied nuclear engineering subjects like neu-
tronics, reactor thermal-hydraulics, reactor safety analysis, reactor operation principles, radiation protection, etc. He graduated with a top 2 GPA in a class of 60 students.

In 2001, he was admitted to the graduate program of Institute of Nuclear Engineering Technology (INET) at Tsinghua University (China) without having to take the entrance exams. He took some graduate level courses like advanced neutronics, reactor engineering, computational methods, etc. and did some research on public acceptance on nuclear energy. During his stay in Beijing, he met his future wife and got married in 2003. He left INET when he found the program did not match his goals.

In 2003, he became a graduate student of University of Illinois at Urbana-Champaign (UIUC) in nuclear engineering under the advising of Prof. Rizwan-uddin. He took a few courses to fulfil the PhD degree requirement and also to facilitate his research. First he worked on UIUC TRIGA reactor and developed a detailed reactor model using MCNP. Then he spent some time on the Virtual Reality project to help render 3D models on the CUBE system. He then focused on the simulation and modification of Australian Open Pool Light-water reactor (OPAL) for advanced research reactor design. He received his M.S. in May 2006 and he is looking forward to receiving his PhD in May 2011.

While he is a PhD student of UIUC, he found a student position at Los Alamos National Laboratory (LANL) and moved his family to Los Alamos, New Mexico in 2007. He first worked in the Theoretical Division under the mentoring of Dr. Anna Hayes, then he transferred to the Nuclear Nonproliferation Division (N-4) under the mentoring of Dr. Stephen Tobin. After completing his PhD, he will continue to work at N-4 at LANL.