Monte Carlo and analytical calculations of the Dancoff Factor in Pebble Bed Reactors, specifically for Wallpaper Fuel and Moderator Pebbles

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Abstract

The pebble bed reactor is one of the generation IV nuclear reactor designs that is globally investigated for future nuclear power plants. It allows for passive safety and less nuclear waste production. When analysing the pebble bed reactor, the Dancoff factor appears in the calculation of group-wise resonance shielded cross sections due to resonance neutrons being able to enter fuel lumps adjacent to the one they originated in. This Dancoff factor has often been investigated for regular pebbles, but only very little for wallpaper fuel and dummy pebbles. Therefore the Dancoff factor in these two types of pebbles is the main focus of this research.

Two Monte Carlo based codes were developed for the numerical calculation of Dancoff factors as a function of various design parameters, specifically for wallpaper and dummy pebbles. The first, MCDancoff-PB, generates a complete pebble bed configuration in order to simulate neutron flight paths and calculate the Dancoff factor. This code was first used to determine the dependence of the Dancoff factor for regular pebbles to several design parameters, such as the TRISO packing fraction and the number of TRISO particles. The Dancoff factor for regular pebbles was found to increase for increasing TRISO packing fractions and higher numbers of TRISO particles, conform other research.

Wallpaper fuel is interesting due to its favourable temperature characteristics. The Dancoff factor was calculated for wallpaper fuel using MCDancoff-PB and was found to follow the same trends as for regular pebbles when increasing the TRISO packing fraction or number of TRISO particles. The Intra Dancoff factor was shown to decrease when increasing the central fuel free zone radius up to half the fuel zone radius, and to increase for larger central fuel free zone radii up to 0.9 times the fuel zone radius. After this maximum it decreases again. The Inter Dancoff factor therefore varies only slightly for small central fuel free zone radii and increases significantly for radii larger than half the fuel zone radius. The maximal difference measured between the Dancoff factors for regular fuel and wallpaper fuel was 10%, providing the possibility to approximate the Dancoff factor for wallpaper fuel with that for regular fuel, especially for small central fuel free zone radii.

Dummy pebbles are added to a pebble bed when more moderator volume is required. The fraction of dummy pebbles was shown to influence the Inter Dancoff factor linearly. The Inter Dancoff factor multiplied by the fraction of normal pebbles approximates the actual Inter Dancoff factor to within 5%. This largest error occurs for pebble beds containing as many dummy pebbles as normal pebbles. Combined with the maximal contribution of 20% of the Inter Dancoff factor to the total Dancoff factor, this results in a maximal error of 1% in the total Dancoff factor. The observed linear relation was used to modify the analytical formula proposed by Bende et al. to be applicable to pebble beds containing dummy pebbles. The Dancoff factor calculated by the resulting modified analytical formula is accurate to approximately 3%, an error more than twice as low as with the shell expansion method in the original formula, which is often suggested for dealing with dummy pebbles. The resulting error in the multiplication factor is approximately 1% for this method, using results from Kim et al.. When this accuracy suffices, the modified analytical formula is a much faster alternative to numerical methods.

A second code, MCDancoff-WBC, was developed to verify the steps taken by Bende et al. in deriving their analytical formula. Here a single pebble is generated, incorporating a white boundary condition along its outer surface. One of the steps taken was shown to yield slightly inaccurate results, namely approximating the direction of the neutrons when entering or leaving the fuel zone boundary as a cosine distribution. Other approximations such as using only one pebble with a white boundary along its outer surface were found to produce satisfying results. Without approximating the direction of the neutrons when entering or leaving the fuel zone boundary as a cosine distribution, MCDancoff-WBC was shown to be an accurate method of numerically calculating the Dancoff factor. It was found to be a faster alternative to MCDancoff-PB, while preserving a very good accuracy.

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Chapter 1 Introduction

Since the nuclear disaster of Fukushima in March 2011, public acceptance of nuclear energy has dropped. This has resulted in for example Germany planning to completely abandon nuclear energy. Furthermore, nuclear waste is accumulating and has to be stored safely for thousands of years to lose most of its radioactivity. Various methods of storing nuclear waste are being investigated, such as geological storage, but none come without risks [1]. These issues pose a great challenge for nuclear energy.

On the other hand, global energy consumption increases rapidly [2] and the need for an inexhaustible and reliable energy source grows larger every year. Fossil fuels, the main source of our energy, become more and more expensive due to their limited supplies and are often related to global warming due to the release of carbon dioxide [3], while the costs of renewable energy are unable to compete using current technologies. Therefore nuclear energy is still considered as a viable alternative, despite the possibility of a disaster with a huge impact on both the environment and the economy. Ample amounts of uranium and thorium, the fuel used in nuclear power plants, are available on this planet and the carbon dioxide emission is comparable to renewable energy.

In order to reduce the problems of safety and nuclear waste, six different designs of nuclear reactors with higher fuel efficiency and improved safety features are internationally being investigated. These designs carry the name of generation IV nuclear reactors [4]. One of these designs is the pebble bed reactor, which is investigated in this research.

1.1 The pebble bed reactor

The pebble bed reactor is a graphite moderated very high temperature nuclear reactor, cooled by gaseous helium. It consists of a reactor vessel lined with graphite reflectors, containing up to half a million randomly stacked spherical fuel elements, called pebbles. These stacked pebbles form a so-called pebble bed. The helium flows through the void in between the pebbles as well as through the graphite reflectors. This primary cooling system can either work a turbine itself, or transport the heat generated inside the pebble bed to a secondary cooling system containing pressurised water, working a steam turbine. Pebbles can be refilled at the top of the pebble bed and extracted at the bottom. This allows for refueling during reactor operation. A schematic overview of a pebble bed reactor is shown in figure 1.1.

Two types of pebbles are considered for the pebble bed reactor. Only one of these has also been constructed, and is currently in use in the HTR-10 prototype in China [6]. This 'regular' pebble is composed of a 5 cm diameter fuel zone surrounded by a 5 mm thick graphite shell. The fuel zone is filled with thousands of randomly stacked TRISO particles embedded in a graphite matrix. These TRISO particles are small fuel kernels with a diameter of approximately 500 μ m, made of for example uranium dioxide, surrounded by four layers of coatings with a total thickness of typically 200 μ m to contain the radioactivity. The other type of pebble is called the wallpaper pebble and has a similar design, but contains a central fuel free zone of graphite with a diameter



Figure 1.1: A schematic overview of a pebble bed reactor [5].



Figure 1.2: Regular fuel and wallpaper fuel considered for the pebble bed reactor.

of typically 4 cm. This graphite may be of a different density than the other graphite used in the pebble, but not necessarily. The design of wallpaper fuel is mainly under investigation to lower the peak temperature of the TRISO particles [7]. Since the heat is generated near the pebble outer shell, it is more easily transported out of the pebble. Both types of pebbles are shown in figure 1.2. A third type of pebble made of only graphite, called a moderator pebble or dummy pebble, is often added to the pebble bed when extra moderator volume is required.

The pebble bed reactor has several advantages over earlier generation nuclear reactors. Most importantly, it can be inherently safe if designed correctly [10]. A low power density ensures sufficient heat transfer if a loss of cooling event occurs. Passive mechanisms such as heat radiation, conduction and convection of the helium coolant provide enough cooling to prevent a core meltdown. Moreover, the TRISO coating layers retain both fuel and fission products below 1600 degrees Celsius, preventing significant radiation release to the environment. These passive safety features were successfully tested with the HTR-10 prototype in China [6].

Another major advantage is the possible reduction of nuclear waste. A pebble bed reactor can be operated as a thorium breeder or plutonium burner [11]. Thorium has a lower mass than the conventionally used uranium and therefore produces significantly fewer long-lived heavy actinides. Moreover, the heavy actinides that are still produced, such as plutonium, can be burned, leaving only fission products as nuclear waste. These fission products have a much shorter lifetime than the heavy actinides. Already after several hundreds of years they generally produce less radiation than naturally occurring isotopes. Besides burning heavy actinides which are created during operation, it is also possible to introduce extra heavy actinides in the fuel for burning. This allows for the disposal of currently stored heavy actinides, thus reducing the nuclear waste from earlier generation nuclear reactors. Finally, the helium coolant and graphite moderator allow for higher temperatures than water moderated and cooled reactors, increasing the thermal efficiency.

Of course the pebble bed reactor, since it is still under design, requires further testing for safety and waste management [12]. Core temperatures exceeding 1600 degrees Celsius cause the detention capability of the TRISO coating layers to decrease significantly, no longer preventing significant radiation release to the environment. This temperature must therefore be shown never to be exceeded. Furthermore, the nuclear waste produced is encapsulated within graphite, complicating the recycling of spent fuel. Storage of the pebbles without any form of reprocessing is also considered, but increases the volume of the nuclear waste significantly. Finally, just like any other nuclear reactor, the reactor core needs to be encapsulated within a protective vessel to deal with the threats of natural disasters and acts of terrorism. Nevertheless, in a world with growing concerns about the safety of nuclear energy, the pebble bed reactor provides a very good prospect.

1.2 The Dancoff factor

In a nuclear reactor, neutrons released by fission slow down to lower energies by suffering moderator collisions. During this process, they experience an appreciable probability of being absorbed by capture resonances in heavy nuclei such as uranium-238 or thorium-232 [13]. A capture resonance is a very large peak in the capture cross section, increasing the neutron capture probability. These absorptions, also known as resonance shielding, are extremely important in nuclear reactors, because they affect numerous reactor characteristics. Usually when treating this resonance shielding, fuel lumps are treated as if they are isolated from other fuel lumps. This is true when the distance between fuel lumps is many mean free path lengths long. For pebble bed reactors however, this is not the case. Fuel lumps in a pebble bed reactor are typically separated by distances in the order of a single mean free path length.

This is where the Dancoff factor arises. Usually the probability that a neutron escapes from a fuel lump, called the first-flight escape probability and used in the calculation of group-wise resonance shielded cross sections, implies that the neutron suffers its next collision in the moderator. When other fuel lumps are nearby however, this collision may also occur in the fuel. The first-flight escape probability must therefore be corrected by the probability that a neutron escaping a fuel lump will enter another fuel lump, also referred to as the 'shadowing effect'. This probability is called the Dancoff factor [14].

The Dancoff factor in a pebble bed reactor is complicated due to the double heterogeneity of the system. First of all there are thousands of coated fuel kernels in a pebble, which is the first heterogeneity. Then there are also thousands of coated fuel kernels in other pebbles, which need to be considered as well. All the pebbles with their graphite outer shells form the second heterogeneity. Due to this double heterogeneity, the Dancoff factor in a pebble bed is often split up in two parts, which are separately calculated. The first part is the Intra Dancoff factor, denoting the probability that a neutron escaping a fuel kernel will enter another fuel kernel in the *same* pebble The second part is the Inter Dancoff factor, which is the probability that a neutron escaping a fuel kernel will enter another fuel kernel in *another* pebble. Adding up these probabilities yields the total Dancoff factor.

Some previous studies of the Dancoff factor are quickly summarised here. Lane et al. [15] derived an expression for the infinite medium Dancoff factor for randomly distributed particles in 1962. This infinite medium Dancoff factor is acquired by filling all space with only TRISO particles embedded in a graphite matrix and neglecting the second heterogeneity. Janssen [16] adjusted the cross sections in this model by the volume fraction occupied by the fuel kernels for slightly more accurate results in 1990. Bende et al. [17] derived an analytical formula for the Dancoff factor in 1999 based on a two-region white boundary unit cell for even better results. Kloosterman and

Ougouag [18] compared all these methods to Dancoff factors calculated by two computer codes, INTRAPEB and PEBDAN, in 2007. These codes were found to yield very accurate results, but also require more computation time than the analytical methods. Ji and Martin [14] successfully applied chord length probability density functions to find analytical expressions for the Dancoff factor in 2011. Kim et al. [19] used another numerical method to accurately calculate Dancoff factors in 2012.

1.3 Research outline

In the mentioned studies, much attention was paid to the Dancoff factor for regular pebbles. Dummy pebbles were however often neglected or dealt with by methods which were not verified. Moreover, wallpaper fuel is investigated for its temperature characteristics, for example in the work of Marmier et al. [7], but the Dancoff factor is considered only briefly and the methods used to calculate it are unclear.

Therefore, a new Monte Carlo code, MCDancoff-PB, is written to numerically evaluate the Dancoff factor for various design parameters. Most importantly, it is capable of implementing wallpaper fuel and dummy pebbles. The results for regular pebbles are compared to existing methods such as the analytical formula proposed by Bende et al. [17] and the numerical results from Kim et al. [19] to verify the method. Using MCDancoff-PB the dependence of the Dancoff factor for regular pebbles to several parameters is then investigated as reference data, followed by the differences occurring when wallpaper pebbles are used and when dummy pebbles are added.

An accurate analytical formula for the Dancoff factor is highly desirable, because this requires much less computation time than numerical methods. The analytical formula proposed by Bende et al. [17] was shown to be accurate to approximately 2% by Kloosterman and Ougouag [18]. Another Monte Carlo code, MCDancoff-WBC, is written to numerically verify the steps taken by Bende et al. in deriving their analytical formula and find the cause of any errors occurring in their results. Moreover, MCDancoff-WBC is also designed as a faster alternative for MCDancoff-PB. Based on the numerical results for dummy pebbles, the analytical formula proposed by Bende et al. is slightly modified to be applicable to pebble bed configurations containing dummy pebbles using a more accurate method than considered before.

Chapter 2 briefly covers the theoretical background necessary to understand the physics behind Dancoff factors. Chapter 3 provides a detailed description of both MCDancoff-PB and MCDancoff-WBC. Chapter 4 shows Dancoff factors computed by both codes as well as the modified analytical formula. Based on these results some conclusions are drawn. All conclusions are summarised and accompanied by recommendations for future research in chapter 5. This research was conducted as a Bachelor Thesis at the Delft University of Technology.

Chapter 2

Theory

The theoretical background necessary to understand the physics behind Dancoff factors is briefly covered here. As a starter some basic knowledge on nuclear reactor physics is provided. This knowledge is then used to formally introduce the Dancoff factor. Some attention is paid to the analytical formula proposed by Bende et al. [17] as well.

2.1 Basics of nuclear reactor physics

The basics of nuclear reactor physics relevant to the numerical calculation of the Dancoff factor mainly consist of nuclear cross sections, which are of great importance for dealing with neutron interaction probabilities, and of resonance shielding, in which the Dancoff factor arises. Nuclear fission and reactor criticality are also covered, since these are essential for operating a nuclear reactor and the multiplication factor, used to determine the reactor criticality, is affected by the Dancoff factor.

2.1.1 Cross sections

The nuclear cross section characterises the probability that an interaction between a neutron and a nucleus will occur [13]. When dealing with a separate nucleus, or a very thin layer of nuclei, the microscopic cross section σ is defined as:

$$\sigma = \frac{\text{Number of reactions / nucleus / s}}{\text{Number of incident neutrons / cm2 / s}}$$
(2.1)

This microscopic cross section depends upon the type of interaction, the type of nucleus and the energy of the incident neutron. Common examples of interactions between neutrons and nuclei are scattering (σ_s), radiative capture (σ_γ) and fission (σ_f). It is often convenient to look at the total microscopic cross section (σ_t) instead of specific ones. Since microscopic cross sections are essentially probabilities, they can simply be added up to produce a total:

$$\sigma_t = \sum_i \sigma_i = \sigma_s + \sigma_\gamma + \sigma_f + \cdots$$
(2.2)

In nuclear reactors, neutrons are incident upon a complete slab of material instead of a single nucleus. In this case, the macroscopic cross section is used and defined as:

$$\Sigma_t = N\sigma_t \tag{2.3}$$

Here N denotes the number density of the target nuclei. The unit of Σ_t is cm⁻¹, no longer in line with the term cross section. It is however still related to interaction probabilities. The probability that no interaction occurs when a neutron travels a distance x through the target material is given by:

$$P(\text{no interaction}) = e^{-\Sigma_t x} \tag{2.4}$$

This probability is of great importance when calculating Dancoff factors, as is further explained in section 3.1.2.

2.1.2 Nuclear fission

When a neutron is incident upon a nucleus, several types of interactions may occur. The probability of a certain interaction occurring was shown to be related to the nuclear cross section in the previous section. One of these possible interactions is nuclear fission, which is the principle behind any (existing) nuclear reactor. A fissionable nucleus may split into two smaller nuclei when interacting with an incident neutron, releasing a large amount of energy and several new neutrons [13]. These new neutrons may themselves cause another nucleus to split, causing a chain reaction. This process is schematically shown in figure 2.1.



Figure 2.1: A nuclear fission chain reaction [20].

Not all elements are fissile (fissionable by thermal neutrons) and usable in a nuclear reactor. This is related to the binding energy of a nucleus. The combined mass of separate nucleons (protons and neutrons) that make up a nucleus is usually larger than the mass of the nucleus itself. The mass defect that occurs has been converted to potential energy when the nucleus was formed to stabilise the bond and is called the binding energy. The binding energy per nucleon as a function of the atomic mass is shown in figure 2.2. For light elements the binding energy increases a lot with an increasing atomic mass. They therefore release a lot of energy when fused. This increase ends with Fe-56, which has the highest binding energy per nucleon of all elements. For even heavier elements, the binding energy decreases again. Therefore, these elements release energy when they are split into smaller elements with a higher binding energy. This is the energy that is released with nuclear fission. Other factors such as the cross section for fission also affect whether an element is usable in a nuclear reactor. Therefore only a small subset of elements is used in practice.



Figure 2.2: The binding energy per nucleon as a function of the atomic mass [21].

2.1.3 Reactor criticality

A chain reaction such as described in the previous section is necessary to operate a nuclear reactor. The multiplication factor k_{eff} gives information about the growth of the chain reaction. It is defined as the number of neutrons in one generation as compared to the number of neutrons in the previous generation by [13]:

$$k_{eff} = \frac{\text{Number of neutrons in one generation}}{\text{Number of neutrons in preceding generation}}$$
(2.5)

In order to sustain the chain reaction at a certain level, a k_{eff} of 1 is required. If this is the case, the reactor is called critical and a constant amount of energy is produced. This is of course aimed for to safely and effectively operate a nuclear reactor. If k_{eff} is smaller than 1, the number of reactions occurring per time unit is reducing and the chain reaction diminishes. The reactor is then called subcritical. This occurs for example when shutting the reactor down. If k_{eff} exceeds 1, more neutrons are inducing fission reactions in every succeeding cycle. The reactor is then called supercritical. A reactor is made slightly supercritical when starting up. An example of a very supercritical situation is an atomic bomb, in which case the chain reaction is meant to grow as explosively as possible. The Dancoff factor affects this multiplication factor and is therefore important for operating a nuclear reactor.

2.1.4 Resonance shielding

It was already mentioned in section 2.1.1 that cross sections depend on the energy of the incident neutron. Neutrons released in a fission reaction usually have a high energy (fast neutrons) for which the fission cross section is very small. In order to increase the chance for them to induce a fission reaction in another target nucleus, they need to be slowed down by the moderator. While slowing down however, they have an appreciable probability of being absorbed by capture resonances in heavy nuclei such as uranium-238 or thorium-232 [13]. A capture resonance is a very large peak in the capture cross section, increasing the neutron capture probability. For neutron energies of 1-100 eV the cross section of Uranium-238 for example exhibits some very large resonance peaks, which is shown in figure 2.3.

In order to minimise non-fission capture, the fuel and moderator are usually placed in different regions in the reactor core. This way, a fast neutron created by a fission reaction, which has only a small probability of being absorbed in the fuel, often escapes the fuel region and enters the moderator region. The neutron then slows down inside the moderator region, preferably all the way to thermal energies (< 0.01 eV), before entering the fuel region again. Thermal neutrons have a large probability of inducing a fission reaction, due to the high cross section for fission



Figure 2.3: Absorbtion cross sections for uranium-238 [22].

of uranium-235 in this energy range. Of course neutrons may enter the fuel region after only a few moderator interactions when their energy is still well above the thermal range. They then have a significant probability of being caught by resonance absorption. This situation is called self-shielding or resonance shielding of the fuel.

The probability that a neutron escapes a fuel lump and suffers its next interaction in the moderator, P_{FM} , is very important in a nuclear reactor. It is used in the calculation of group-wise resonance shielded cross sections. P_{FM} needs to be high to assure that many neutrons are slowed down to thermal energies, in order to be likely to induce a fission reaction. Resonance shielding however significantly reduces P_{FM} . If the fuel lumps are isolated, P_{FM} is given by the first-flight escape probability P_{esc} , since neutrons escaping a fuel lump have to travel many mean free path lengths through the moderator region before crossing a fuel lump again and can therefore be expected to suffer a moderator collision. For a sphere, such as a fuel kernel, P_{esc} is given by [23]:

$$P_{esc}(E) = \left(\frac{3}{8\lambda^3}\right) \left[2\lambda^2 - 1 + (1+2\lambda)\exp(-2\lambda)\right]$$

$$\lambda = r_{\rm T} \Sigma^F$$
(2.6)

Here r_F denotes the radius of the fuel kernel and Σ_t^F the total macroscopic cross section of the fuel. From equation 2.6 it is clear that for higher total macroscopic cross sections of the fuel, for example due to resonance absorption of 1-100 eV neutrons, the escape probability reduces.

2.2 The Dancoff factor

In a pebble bed, fuel lumps are not isolated. They are typically separated by distances in the order of a single mean free path length. There is therefore a significant probability that a neutron escaping a fuel kernel will not suffer its first interaction in the moderator. Taking into account the double heterogeneity, there is a probability that the neutron will enter another fuel kernel in either the same pebble or in another pebble. This probability is called the Dancoff factor (C) [14]. P_{FM} is now slightly more complicated, but can still be expressed as P_{esc} , corrected using the Dancoff factor [18]:

$$P_{FM} = P_{esc} \frac{1 - C}{1 - C(1 - P_F)}$$
(2.7)

Here P_F is the probability that the neutron suffers its first interaction in a fuel kernel, which is of course relevant when the neutron has entered one. It is evident from equation 2.7 that P_{FM} is reduced by the correction factor. The Dancoff factor leads to increased self-shielding of the fuel and is therefore sometimes referred to as the "shadowing effect" [14]. It is mostly evaluated for neutron energies of 10-100 eV due to most of the resonance absorption of uranium-238 in this region. Moreover, the graphite total cross section only varies slightly for this energy range, considerably simplifying Dancoff factor calculations.

The Dancoff factor affects the multiplication factor discussed in section 2.1.3. Kim et al. [19] showed that a decrease of 10% in the Dancoff factor can decrease k_{eff} by 3.7%. The Dancoff factor is therefore of significant importance for properly designing a pebble bed reactor. These numbers however do implicate that a certain error in the Dancoff factor is of less influence to the error in the multiplication factor, thus allowing for a small error in the Dancoff factor to still yield accurate results for k_{eff} .

2.3 The analytical formula proposed by Bende et al.

Bende et al. [17] derived an analytical formula for the Dancoff factor that yields results accurate within approximately 2% [18]. This accuracy can be sufficient for various purposes when considering the implications on the error in k_{eff} mentioned in the previous section. It provides a very fast method of calculating Dancoff factors when compared to numerical methods. In their derivation, Bende et al. defined various transmission probabilities for neutrons in both heterogeneous systems involved. These are the fuel kernel with its coating layers and the pebble fuel zone with its graphite shell. They presumed that the fuel zone was completely filled with TRISO particles, adding the graphite matrix in which they are embedded to the coating layers. The transmission probabilities used here are listed in table 2.1 and shown in figure 2.4. Some extra information is also present in figure 2.4 that was used for the derivation of the analytical formula and that is not discussed here. The interested reader is invited to read the original paper by Bende et al. [17] for the full derivation.

probability t_{io} Probability that a neutron isotropically leaving the fuel kernel boundary reaches the outer coating boundary without collisions. t_{oi} Probability that a neutron isotropically leaving the outer coating bound- ary reaches the fuel kernel boundary without collisions. t_{oo} Probability that a neutron isotropically leaving the outer coating bound- ary reaches again the outer coating boundary without collisions and without passing through the fuel kernel
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without passing through the fuel kernel
without passing through the fuel kernel.
t_{ii} Probability that a neutron isotropically leaving the fuel kernel bound-
ary (directed inward) reaches again the fuel kernel boundary without
collisions and without leaving the fuel kernel.
T_{IO} Probability that a neutron isotropically leaving the pebble fuel zone
boundary reaches the outer shell boundary without collisions.
T_{OI} Probability that a neutron isotropically leaving the outer shell boundary
reaches the pebble fuel zone boundary without collisions.
T_{OO} Probability that a neutron isotropically leaving the outer shell boundary
reaches again the outer shell boundary without collisions and without
passing through the pebble fuel zone.
T_{II} Probability that a neutron isotropically leaving the pebble fuel zone
boundary (directed inward) reaches again the pebble fuel zone boundary
without collisions and without leaving the pebble fuel zone.

Table 2.1: Transmission probabilities defined by Bende et al. [17].



(b) The pebble fuel zone with its graphite shell, containing TRISO particles.

Figure 2.4: Transmission probabilities defined by Bende et al. [17].

Using the transmission probabilities from table 2.1 and figure 2.4, Bende et al. derived an infinite medium Dancoff factor for both the fuel kernel (C_{∞}^{fk}) and the pebble fuel zone (C_{∞}^{FZ}) :

$$C_{\infty}^{fk} = \frac{t_{io}t_{oi}}{1 - t_{oo}} \tag{2.8}$$

$$C_{\infty}^{FZ} = \frac{T_{IO}T_{OI}}{1 - T_{OO}} \tag{2.9}$$

Of course both the fuel kernel and the pebble fuel zone are not of infinite dimensions. Therefore a correction factor was derived to account for the finite geometry involved in a pebble bed. First of all, they split the Dancoff factor into two separate parts to account for the double heterogeneity involved: the Intra Dancoff factor (C_{intra}) , denoting the probability that a neutron leaving a fuel kernel enters another fuel kernel in the *same* pebble, and the Inter Dancoff factor (C_{inter}) , denoting the probability that a neutron leaving a fuel kernel enters another fuel kernel in another pebble. These are of course added up to calculate the total Dancoff factor:

$$C = C_{intra} + C_{inter} \tag{2.10}$$

The final equation they arrived at to calculate the Dancoff factor analytically then is given by:

$$C_{intra} = C_{\infty}^{fk} \left[1 - P_F \left(\Sigma^* R_{fuelzone} \right) \right]$$
(2.11)

$$C_{inter} = C_{\infty}^{fk} C_{\infty}^{FZ} \frac{P_F \left(\Sigma^* R_{fuelzone} \right) [1 - T_{II}]}{1 - T_{II} T_{IO} T_{OI}}$$
(2.12)

$$C = C_{\infty}^{fk} \left[1 - P_F \left(\Sigma^* R_{fuelzone} \right) + C_{\infty}^{FZ} \frac{P_F \left(\Sigma^* R_{fuelzone} \right) \left[1 - T_{II} \right]}{1 - T_{II} T_{IO} T_{OI}} \right]$$
(2.13)

Here P_F is again the probability that a neutron suffers its first interaction in a fuel kernel and Σ^* is the pseudo cross section, the total moderator cross section corrected for the probability that a neutron will enter a fuel kernel. It can be interpreted as the probability per unit path travelled that a neutron will either collide with a moderator nucleus or enter a fuel kernel and is given by:

$$\Sigma^* = \left(\frac{-\ln t_{oo}}{\bar{l}_{TRISO}}\right) \tag{2.14}$$

Here \bar{l}_{TRISO} is the average distance a neutron travels in the first TRISO particle it originated in and in the final TRISO particle where it either enters a fuel kernel or suffers a moderator collision. When discussing the results of this research, equation 2.13 is often referred to. The steps taken in deriving equation 2.13 are also numerically tested in section 4.2. Moreover, in section 4.3 equation 2.13 is slightly modified to be applicable to pebble bed configurations containing dummy pebbles.

Chapter 3 FORTRAN codes

To calculate the Dancoff factor numerically, two different Monte Carlo approaches are followed and implemented into a FORTRAN code. First a reference case is set up in which a complete pebble bed is generated in order to simulate neutron flight paths as closely to reality as possible, resulting in the FORTRAN code MCDancoff-PB. This approach will be shown to yield accurate and reliable results, but also takes a lot of computation time. The second approach, implemented in the FORTRAN code MCDancoff-WBC, is an adapted form of the method used by Bende et al. [17], which only requires a single pebble to be generated and incorporates a white boundary condition along its outer surface. This method requires significantly less computation time, but several approximations are made which need to be validated.

3.1 MCDancoff-PB

MCDancoff-PB consists of two separate parts. First a cylindrical pebble bed configuration is created and then neutron flight paths are simulated in order to calculate the Dancoff factor. After a detailed code description some attention is paid to the uncertainty in the calculated Dancoff factor and validation of the code.

3.1.1 Pebble bed configuration

First a randomly packed pebble bed is generated using the expanding system method by Auwerda et al. [24]. The resulting pebble coordinates are then used as input for MCDancoff-PB. Subsequently each pebble is either listed as a dummy pebble or a fuel pebble, in the latter case followed by assigning a pregenerated set of TRISO coordinates to the pebble. A random configuration of TRISO particles in the pebbles is chosen to reflect the physical situation as well as possible. Since MCDancoff-PB is used for pebble beds containing up to 67,500 pebbles, it is impractical to generate a unique set of TRISO coordinates for each pebble. Instead, 32 unique sets of TRISO coordinates are randomly assigned to the fuel pebbles. This approach is supported by both physical arguments and simulation results in section 3.1.4.

To create the TRISO coordinates within a pebble, a point is randomly generated within a cube and then tested to be suitable as center of a TRISO sphere. This means that the complete TRISO particle must be located within the pebble fuel zone and have no overlap with other TRISO particles. For wallpaper fuel, the complete TRISO particle must also be located outside of the fuel-free central area of the pebble. If all conditions are met, the point is accepted and the process is repeated until all the TRISO coordinates are generated. The number of points that is rejected increases as the pebble fuel zone becomes more densily packed with TRISO particles. Therefore the time needed to create the TRISO coordinates strongly depends upon the desired

TRISO packing fraction, calculated by:

$$pf = N_{TRISO} \left(\frac{(R_{kernel} + D_{coating})}{R_{fuelzone}} \right)^3$$
(3.1)

This algorithm works well for TRISO packing fractions up to approximately 32%. That is well below the maximal achievable 62% for randomly packed beds, but sufficient for practical situations, which are the main focus of this research.

Multiple unique sets of TRISO coordinates are created and written in files in order to save time for subsequent calculations. These are then, as mentioned before, assigned to the pebbles, which concludes the pebble bed generation. For simplicity and efficiency reasons the coating layers surrounding the fuel kernels are only explicitly added while generating the TRISO coordinates. While simulating the neutron flight paths they are homogeneously mixed with the graphite matrix embedding the TRISO particles. The resulting cross section is approximated as the graphite total cross section, since the coating layers mainly consist of graphite themselves. The input parameters that are related to the pebble bed configuration can be found in table 3.1, namely the pebble radius R_{pebble} , the pebble fuel zone radius $R_{fuelzone}$, the fuel kernel radius R_{kernel} , the TRISO coating thickness $D_{coating}$, the graphite total cross section Σ_t and the neutron mean free path \bar{l} respectively. The graphite total cross section applied here is taken a constant and corresponds to 10-100 eV neutrons, an energy range for which the graphite total cross section varies only slightly. The pebble bed radius and height are omitted, since the calculated Dancoff factor was found to be independent of the pebble bed dimensions due to the generation of neutrons only far away from the pebble bed boundaries, as will be discussed more thoroughly in section 3.1.4.

Table 3.1: Pebble bed related input parameters.

Parameter	Value
R_{pebble}	$3.0~{\rm cm}$
$R_{fuelzone}$	$2.5~\mathrm{cm}$
R_{kernel}	$250~\mu{ m m}$
$D_{coating}$	$200~\mu{ m m}$
Σ_t	$0.41 \ {\rm cm}^{-1}$
$\bar{l} = \Sigma_t^{-1}$	$2.44~\mathrm{cm}$

3.1.2 Neutron path simulation

After the pebble bed geometry has been generated, the Dancoff factor is calculated according to its definition, which is nicely explained in the work of Ji and Martin [14]: the probability that a neutron leaving a fuel kernel will enter another fuel kernel, either in the same pebble (Intra Dancoff factor) or in another (Inter Dancoff factor), without any moderator collisions in between. This is accomplished by generating a number of neutrons in fuel kernels randomly throughout the reactor and following them until they either enter another fuel kernel or suffer a moderator collision. The generation of these neutrons and the simulation of their flight paths will be discussed in detail, followed by a schematic overview in figure 3.2.

The neutrons are generated by randomly selecting a point in a cube with sides twice the fuel kernel radius and then checking if the point is within the fuel kernel sphere. If so, the neutron is accepted and both a pebble (which is not listed as a dummy pebble) and a TRISO particle within this pebble are randomly chosen as starting point for the neutron. Neutron leakage at the pebble bed boundaries must be reduced in order to study the dependence of the Dancoff factor to other parameters more closely. Therefore, neutrons are only generated in pebbles in the middle of the pebble bed, a cylindrical area with half the radius and half the height of the complete pebble bed as shown in figure 3.1. Formally the distance to the pebble bed boundaries should be reduced by the same amount everywhere, but this strategy yields satisfying results for all sizes of pebble beds

studied. This approach is analogous to dictating infinite pebble bed dimensions. The influence of neutrons generated near the pebble bed boundaries is studied in section 3.1.4 to support this approach. Neutron directions are distributed isotropically. Since the Dancoff factor is based on a neutron *leaving* a fuel kernel, the neutron is placed on the fuel kernel shell along the direction of propagation before the flight path simulation starts.



Figure 3.1: Definition of the cylindrical area in the middle of the pebble bed.

Three different areas through which the neutrons pass can be distinguished. These are the pebble fuel zone, the pebble graphite shell and the helium coolant between pebbles. Collisions in the graphite moderator are ignored for now and will be discussed later on. A neutron flight path simulation evidently starts within the pebble fuel zone. Here it is checked whether any fuel kernels lie along the path of propagation of the neutron. If so, the neutron will enter the nearest fuel kernel, which adds to the Intra Dancoff factor. If not, the neutron is placed on the fuel zone shell. The next area to pass through is the pebble graphite shell. The only possibility for the neutron here is to penetrate through the shell and escape the pebble, after which it finds itself inside the helium coolant. Depending on the position of the neutron within the reactor core and its direction of propagation, it has the option to either leak out of the pebble bed through the sides or the top or bottom or enter another pebble. If the neutron leaks out of the pebble bed the neutron flight is aborted. No graphite reflectors have been placed at the pebble bed boundaries, since a (moderator) interaction is needed for the neutrons to be reflected, which then according to the definition makes them ineligible to count for the Dancoff factor. If the neutron enters another pebble it is back in the pebble graphite shell (of another pebble), but it now has two options. Either its direction of propagation is such that it enters the pebble fuel zone, or it will miss the fuel zone and escape the pebble again. In the case of entering the pebble fuel zone it is checked, similar to the method used at the start of the neutron flight path simulation, whether any fuel kernels lie along the path of propagation. Upon entering a fuel kernel the neutron is now counted for the Inter Dancoff factor. Other than that the process repeats itself. If the neutron leaves the pebble without entering the fuel zone, the neutron is back in the helium coolant and the same steps are followed. The only exception to this scheme comes from pebbles listed as dummy pebbles, in which case the neutron simply flies through without having the possibility of entering any fuel kernel.

Along every trajectory within the graphite moderator, the neutrons may suffer moderator collisions. Upon colliding with a moderator (graphite) nucleus, the neutron flight is aborted by simply starting the next neutron flight path simulation and the neutron is not counted for the Dancoff factor. Every time a neutron travels through graphite within the pebbles, there is a chance that a collision will occur. This probability is, analogous to equation 2.4, given as a function of the distance traveled l by:

$$P(interaction) = 1 - e^{-\Sigma_t l} \tag{3.2}$$

Neutron flights are aborted according to this probability during the flight path simulations by comparison with a random number. Inside the helium coolant the interaction probability has been approximated as zero, since the total cross section of helium for neutron interactions is negligibly small compared to that of graphite.

When all the neutron flight paths have been simulated, finally the Dancoff factor is calculated by simply adding up the Intra and Inter Dancoff factor according to equation 2.10. The complete scheme for simulating neutron flight paths in MCDancoff-PB is schematically depicted in figure 3.2.

3.1.3 Uncertainty

The statistical uncertainty in the Dancoff factor u(C) can be evaluated as a function of the number of neutron flight path simulations N and the number of neutrons actually counting for the Dancoff factor N_{hits} using statistical theory by:

$$u(C) = \frac{\sqrt{N_{hits}}}{N} \tag{3.3}$$

With this uncertainty it can be checked whether results are in good agreement. Suppose two different code runs yield outcome A with uncertainty u(A) and outcome B with uncertainty u(B). These results are then said to agree if the absolute difference d obeys:

$$d < 2u(d)$$

$$d = |A - B|$$

$$u(d) = \sqrt{u(A)^2 + u(B)^2}$$
(3.4)

This relation will be used to verify various approximations made in the code. The number of neutron flight path simulations is chosen constant at 1,000,000 for each code run to facilitate the comparison of results.

3.1.4 Code validation

Both the approximations made while building MCDancoff-PB and the Dancoff factors calculated by this code need to be validated. First the influence of neutrons generated near the pebble bed boundaries is studied to validate the method of generating neutrons only in the middle of the pebble bed to avoid neutron leakage. Secondly it is verified that a limited number of unique sets of TRISO coordinates to be used inside the pebbles yields accurate results. Finally the Dancoff factors computed by MCDancoff-PB are compared to results calculated using the analytical formula proposed by Bende et al. [17] to test for reliability and accuracy.



Figure 3.2: A schematic overview of MCDancoff-PB.

Influence of neutron leakage

Neutron leakage through the pebble bed boundaries has a negative effect on the Inter Dancoff factor, since fewer neutrons escaping a pebble near one of the boundaries are able to enter another pebble. This effect reduces with increasing pebble bed dimensions, due to a higher volume-to-surface ratio. Inter Dancoff factors for various pebble bed sizes are listed in table 3.2 to support this theory, as computed by MCDancoff-PB. Here neutrons are still generated throughout the entire pebble bed. Regular pebbles containing 10,000 TRISO particles, leading to a packing fraction of 5.83%, were generated using the input parameters from table 3.1. A constant Intra Dancoff factor of 0.2670 ± 0.0005 was found independent of pebble bed size, as expected.

Table 3.2: Inter Dancoff factors for various pebble bed sizes, computed by MCDancoff-PB.

Radius (cm)	Height (cm)	$\frac{\text{Volume}}{\text{Surface}}$ (cm)	C_{inter}
50	120	17.65	0.0572 ± 0.0002
90	80	21.18	0.0577 ± 0.0002
90	160	28.80	0.0579 ± 0.0002
120	160	34.29	0.0584 ± 0.0002
150	160	38.71	0.0585 ± 0.0002

For the smallest pebble bed, containing only 5,005 pebbles, the number of leaked neutrons is also shown in table 3.3. This number is compared to the situation in which neutrons are only generated in the middle of the pebble bed, as shown in figure 3.1, in order to verify that the observed differences in the Inter Dancoff factor are indeed caused by neutron leakage.

Table 3.3: Inter Dancoff factors and leaked neutrons for the smallest pebble bed, computed by MCDancoff-PB, with and without requiring neutrons to be generated in the middle of the pebble bed.

Middle of pebble bed	C_{inter}	Leaked neutrons
no	0.0571 ± 0.0002	30632
yes	0.0641 ± 0.0003	31

Table 3.2 shows that the Inter Dancoff factor increases slightly for increasing pebble bed dimensions. This data, combined with the 30,000 neutrons leaked from the reactor vessel in table 3.3, 3% of all the simulated neutron flight paths, shows that neutron leakage does indeed negatively affect the Inter Dancoff factor. This observation is in line with the results of both Kloosterman and Ougouag [18] and Kim et al. [19], who report a decrease in the spatially dependent Dancoff factor near the pebble bed boundaries due to neutron leakage.

For this reason it was chosen to generate neutrons in the middle of the pebble bed as discussed in section 3.1.2, thus eliminating the influence of the pebble bed dimensions on the Dancoff factor and allowing to study the influence of other parameters more closely. The 31 neutrons that still leaked out of the pebble bed in table 3.3 while requiring neutrons to be generated in the middle of the pebble bed are insignificant compared to the 1,000,000 neutron histories. Furthermore only the smallest pebble bed containing 5,005 pebbles is used for all other calculations, since this requires the least computation time and was proven to yield the same results as the other pebble beds, as shortly mentioned before in section 3.1.1.

Limited number of unique sets of TRISO coordinates

To determine the fluctuations in the Dancoff factor caused by the number of unique sets of TRISO coordinates available to the pebbles (N_{sets}) , Dancoff factors were computed by MCDancoff-PB while varying this parameter. The options investigated as well as the resulting Dancoff factors are listed in table 3.4. These calculations were performed for regular pebbles containing 10,000

TRISO particles per pebble, causing a packing fraction of 5.83%, using the input parameters as listed in table 3.1.

Table 3.4: Dancoff factors computed by MCDancoff-PB for various numbers of unique TRISO configuration sets.

N_{sets}	C_{intra}	C_{inter}	C
∞	0.2670 ± 0.0005	0.0641 ± 0.0003	0.3311 ± 0.0006
100	0.2671 ± 0.0005	0.0643 ± 0.0003	0.3314 ± 0.0006
32	0.2670 ± 0.0005	0.0642 ± 0.0003	0.3312 ± 0.0006
1	0.2681 ± 0.0005	0.0638 ± 0.0003	0.3319 ± 0.0006

Table 3.4 shows that the Dancoff factors calculated for pebbles containing a limited number of unique TRISO configuration sets do not conflict with the Dancoff factor calculated for a unique set of TRISO coordinates in every separate pebble. This supports the suggestion made in section 3.1.1 that it is unnecessary to simulate the exact physical situation. This also seems unnecessary from a physical point of view for two reasons. Most importantly the influence on the Dancoff factor of any pebbles further away than near-neighbours to the pebble which currently contains a neutron is nearly negligible considering the mean free path of neutrons in graphite is comparable to the pebble radius, as can be seen in table 3.1. On top of that the influence on the Dancoff factor of different TRISO configurations within (neighbouring) pebbles reduces as the TRISO packing fraction increases, since this automatically induces a more homogeneous TRISO distribution.

It is however surprising from a physical point of view that the incorporation of a single TRISO configuration already yields satisfying results, especially for such a low packing fraction. Evidently the exact location of all the TRISO particles within a pebble is insignificant for a random TRISO distribution. Even the Intra Dancoff factor, which could significantly deviate from the average value for only a single realisation, shows no discrepancies. To eliminate the influence of chance however it was chosen for further code runs to make 32 unique sets of TRISO coordinates available to the pebbles. This quantity does not have a major negative effect on the computational efficiency of MCDancoff-PB and rules out most of the near-neighbour correlations.

Validation of the results

The approximations made by generating the neutrons in the middle of the pebble bed and using only a limited number of unique sets of TRISO coordinates for all pebbles in MCDancoff-PB have now been validated. It remains to determine how accurate and reliable the computed Dancoff factors are. To this end the results are compared to Dancoff factors calculated by the analytical formula proposed by Bende et al. [17] in table 3.5 and to Dancoff factors computed by Kim et al. [19], using a method very similar to the method used in this research, in table 3.6. This is done for both a low and a moderately high packing fraction (pf) of TRISO particles within regular pebbles and using the input parameters as listed in table 3.1.

Table 3.5: Dancoff factors calculated by the analytical formula proposed by Bende et al. [17] and by MCDancoff-PB for a low and a moderately high TRISO packing fraction.

Method	Input		$\mathbf{Results}$			
	N_{TRISO}	pf~(%)	C_{intra}	C_{inter}	C	
Bende	10,000	5.83	0.2625	0.0611	0.3236	
MCDancoff-PB	10,000	5.83	0.2670 ± 0.0005	0.0642 ± 0.0003	$0.3312 \pm 0.0006 \; (+2.35\%)$	
Bende	50,000	29.16	0.6738	0.0511	0.7249	
MCDancoff-PB	50,000	29.16	0.6692 ± 0.0008	0.0542 ± 0.0002	$0.7234 \pm 0.0009 \; (-0.21\%)$	

Table 3.5 shows that the Dancoff factors computed by MCDancoff-PB are comparable to the results of Bende et al. [17]. Even so, the difference is larger than the error margins dictated

by formula 3.4, especially for the lower TRISO packing fraction. However, the analytical formula proposed by Bende et al. is known to yield slightly inaccurate results and lacks clear error margins. Moreover, Kloosterman and Ougouag [18] found that the analytical formula underestimates the Dancoff factor at low TRISO packing fractions and overestimates the Dancoff factor at high TRISO packing fractions. This is in line with the results in table 3.5. For the lower TRISO packing fraction the Dancoff factor computed by MCDancoff-PB is mildly higher than the analytical one, while for the moderately high TRISO packing fraction it is slightly lower. It is likely that for even higher TRISO packing fractions the computed Dancoff factor will further drop under the analytical solution, but unfortunately MCDancoff-PB only works well for TRISO packing fractions to a maximum of approximately 32% as discussed in section 3.1.1. These results do however give some confidence in MCDancoff-PB.

Table 3.6: Dancoff factors calculated by Kim et al. [19] and by MCDancoff-PB for a low and a moderately high TRISO packing fraction.

Method	Input		$\mathbf{Results}$			
	N_{TRISO}	pf~(%)	C_{intra}	C_{inter}	C	
Kim	15,000	8.75	0.3586 ± 0.0005	0.0672 ± 0.0002	0.4258 ± 0.0005	
MCDancoff-PB	15,000	8.75	0.3589 ± 0.0006	0.0700 ± 0.0003	$0.4289 \pm 0.0007 \ (+0.73\%)$	
Kim	30,000	17.50	0.5349 ± 0.0007	0.0629 ± 0.0001	0.5978 ± 0.0007	
MCDancoff-PB	30,000	17.50	0.5391 ± 0.0007	0.0662 ± 0.0003	$0.6053 \pm 0.0008 \ (+1.25\%)$	

As can be seen in table 3.6, the Dancoff factor computed by MCDancoff-PB for both TRISO packing fractions is slightly larger than that of Kim et al. [19]. According to the difference dictated by formula 3.4 the results do not agree. Especially the Inter Dancoff factor is, in comparison, overestimated by MCDancoff-PB. MCDancoff-PB however requires the neutrons to be generated in the middle of the pebble bed, thus eliminating the effect of neutron leakage and increasing the Inter Dancoff factor. This was not done by Kim et al., although they did not specify the size of their pebble bed. On top of that the Dancoff factors calculated by Kim et al. were found to differ slightly ($\sim 1\%$) from those calculated with the INTRAPEB code by Kloosterman and Ougouag [18], who found an Intra Dancoff factor of 0.540 for the higher TRISO packing fraction. This result is much more in line with the 0.5391 found by MCDancoff-PB. Also, the main focus of this research is to find the behaviour of the Dancoff factor as a function of various parameters, to which end a 1% accuracy will suffice.

3.2 MCDancoff-WBC

To reduce the computation time needed for computing Dancoff factors and to test the accuracy of the method used by Bende et al. a second FORTRAN code was built, MCDancoff-WBC. MCDancoff-WBC requires only a single pebble to be created with a white boundary condition along its outer surface, conform the steps Bende et al. [17] followed deriving their analytical formula. The differences between this approach and the previously discussed reference case from section 3.1 are highlighted here. In section 4.2 these differences and the Dancoff factors computed by MCDancoff-WBC are validated. Some attention is also paid to the decrease in computation time.

The main difference between MCDancoff-WBC and MCDancoff-PB is that the generation of a complete pebble bed is no longer necessary. Instead only a single pebble is used, containing a set of TRISO coordinates generated as described in section 3.1.1. Naturally this requires a lot less computation time, which is evaluated in section 4.2.5. The geometric input parameters used remain unchanged and can be found in table 3.1.

Neutrons are still generated inside a randomly selected fuel kernel and placed on its shell along the direction of propagation. The first step of the neutron flight path simulation remains the same, since the Intra Dancoff factor is not affected by any differences occurring outside the pebble fuel zone. When the neutrons enter the pebble shell, Bende et al. presume for the derivation of their analytical formula that the angle under which neutrons escape the pebble fuel zone obeys a cosine distribution. This angle is sampled upon leaving the pebble fuel zone. In MCDancoff-WBC the direction of propagation of the neutron is preserved inside the pebble shell, as would physically be expected. The difference between these two methods is discussed in section 4.2.2.

When a neutron reaches the pebble outer surface, it is reflected back into the pebble by a white boundary condition, meaning that the neutron direction is sampled from a cosine distribution. This is analogous to entering another identical pebble at the exact same point under a cosine distributed angle. Bende et al. suggested to expand the pebble graphite shell as a homogeneous mixture of graphite and the surrounding helium coolant, but since the helium cross section was neglected in the reference case, it has also been ignored here. After being reflected by the white boundary condition, the neutron either reaches the boundary again, resulting in another reflection, or penetrates the pebble fuel zone in which case the process repeats itself. When all neutrons have either entered another fuel kernel or suffered a moderator collision on the way, the Intra and Inter Dancoff factor are added up according to equation 2.10 to calculate the final Dancoff factor. The number of neutron flight paths simulated remain unchanged at 1,000,000 to facilitate comparison with the reference case.

Dummy pebbles were proposed by Bende et al. [17] to be handled by adding up the volume they represent to the regular pebbles, thus expanding the pebble graphite shell. This procedure allows the analytical formula to be easily applicable to pebble bed configurations containing any amount of dummy pebbles. Incorporation into MCDancoff-WBC revealed however that this routine yields incorrect results, which is supported in section 4.2.4. Therefore another routine was developed, no longer in line with the derivation by Bende et al.. Instead, pebbles are randomly transformed into dummy pebbles as neutrons reflect from the white boundary, with a probability proportional to the relative number of dummy pebbles present inside the pebble bed. This method was found to give very good results, as shown in section 4.2.4. The analytical formula is also slightly modified in section 4.3 to incorporate this approach. A scheme outlining the structure of MCDancoff-WBC is depicted in figure 3.3.



Figure 3.3: A schematic overview of MCDancoff-WBC.

Chapter 4

Results

Dancoff factors calculated by both MCDancoff-PB and MCDancoff-WBC are studied here. Based on these results, several conclusions are drawn and motivated elaborately. All conclusions are summarised in chapter 5. The chapter ends with a slight modification of the analytical formula proposed by Bende et al. [17] to make it applicable to pebble bed configurations containing dummy pebbles.

4.1 MCDancoff-PB

MCDancoff-PB is used to study the influence of several parameters on the Dancoff factor. First, regular pebbles are modelled in order to briefly investigate the influence of the pebble size, the number of TRISO particles and the TRISO packing fraction. Secondly, wallpaper pebbles are modelled and compared to regular pebbles for all possible sizes of the central fuel free zone. Finally, dummy pebbles are added to the pebble bed for both types of pebbles to determine how much they will decrease the Inter Dancoff factor.

4.1.1 Regular pebbles

Much research to the Dancoff factor has been conducted in the past, most of which focuses on regular pebbles. Dependencies of the Dancoff factor to several parameters were already investigated in the research of, among others, Bende et al. [17]. Three of these dependencies for regular pebbles are briefly studied again using MCDancoff-PB to verify the observed trends. These are the influence of the pebble size, the number of TRISO particles and the TRISO packing fraction. The results are mainly meant for comparison with wallpaper fuel in section 4.1.2. It is not possible to change one of these parameters without affecting one of the others, since they relate according to formula 3.1. Therefore Dancoff factors are calculated using MCDancoff-PB while keeping one parameter constant and varying the other two. This is done for the Intra Dancoff factor at first. The results of these calculations can be found in table 4.1. The fuel kernel radius, coating thickness and graphite total cross section are chosen constant at the values listed in table 3.1.

Increasing the TRISO packing fraction in regular pebbles will increase the Intra Dancoff factor, as can be observed from the first two sets of results in table 4.1. The TRISO packing fraction is increased by either increasing the number of TRISO particles or decreasing the pebble fuel zone size. A higher TRISO packing fraction means that neutron path lengths between fuel kernels will decrease, reducing the chance of any moderator collisions. Also, the number of neutron paths crossing another fuel kernel are increased, reducing the amount of neutrons escaping the pebble. The third set of results suggests that the Intra Dancoff can also be increased by increasing the number of TRISO particles while conserving the TRISO packing fraction by increasing the fuel zone volume just as much. Since the TRISO packing fraction remains the same, the average neutron path length and therefore the amount of moderator collisions should not change. The

N_{TRISO}	$R_{fuelzone}$ (cm)	pf~(%)	C_{intra}
10,000	2.5	5.83	0.2670 ± 0.0005
25,000	2.5	14.58	0.4905 ± 0.0007
40,000	2.5	23.33	0.6143 ± 0.0008
50,000	2.5	29.16	0.6692 ± 0.0008
3,000	2.0	3.42	0.1530 ± 0.0004
3,000	1.5	8.10	0.2676 ± 0.0005
3,000	1.0	27.34	0.4965 ± 0.0007
2,500	1.0	22.78	0.4456 ± 0.0007
20,000	2.0	22.78	0.5766 ± 0.0008
67,500	3.0	22.78	0.6296 ± 0.0008

Table 4.1: The Intra Dancoff factor calculated by MCDancoff-PB while keeping either $R_{fuelzone}$, N_{TRISO} or the TRISO packing fraction constant.

chance of neutrons escaping the pebble does however decrease, thus increasing the Intra Dancoff factor. As the fuel zone radius increases, the volume and also the number of TRISO particles increases by a third power. The surface of the fuel zone only increases by a second power. Therefore the fraction of the surface 'filled' by fuel kernels increases, resulting in fewer neutrons escaping the pebble. The combined effect of the TRISO packing fraction and the number of TRISO particles can also be observed in table 4.1. The Intra Dancoff factors for 3,000 TRISO particles are lower than those for comparable TRISO packing fractions, but with more TRISO particles. The Intra Dancoff factor is highest for the highest TRISO packing fraction and for the most TRISO particles. The TRISO packing fraction does however seem to be the major influence on the Intra Dancoff factor. The radius of the pebble fuel zone mainly influences this TRISO packing fraction, and is therefore observed to either increase or decrease the Dancoff factor, dependent on the change in the number of TRISO particles. Although this data is rather limited, the observations are in line with the research of Bende et al. [17] and will not be investigated further.

The Inter Dancoff factor mainly depends upon the thickness of the pebble graphite shell. A thicker shell means more moderator interactions and consequently a lower Inter Dancoff factor. It is affected by the amount of neutrons escaping the pebble as well, since only neutrons escaping the pebble can count for the Inter Dancoff factor. The Inter Dancoff factor as a function of the thickness of the pebble graphite shell was already plotted by Bende et al. [17] and is not investigated here. If the fuel zone radius is increased while preserving the amount of neutrons escaping it, the Inter Dancoff factor for a constant shell thickness will still decrease. This is caused by increased neutron path lengths through the graphite shell when missing the fuel zone. This effect is not investigated either, since only one pebble size ($R_{pebble} = 3 \text{ cm}$) is usually considered for realistic pebble bed reactors. Inter Dancoff factors for a constant fuel zone radius and shell thickness were calculated using MCDancoff-PB and are shown in table 4.2. The input parameters from table 3.1 were used. The Intra and total Dancoff factor are listed as well.

Table 4.2: Inter, Intra and total Dancoff factors calculated by MCDancoff-PB for a constant pebble fuel zone radius and shell thickness.

N_{TRISO}	pf~(%)	C_{inter}	C_{intra}	C
10,000	5.83	0.0642 ± 0.0003	0.2670 ± 0.0005	0.3312 ± 0.0006
25,000	14.58	0.0692 ± 0.0003	0.4905 ± 0.0007	0.5597 ± 0.0007
40,000	23.33	0.0600 ± 0.0002	0.6143 ± 0.0008	0.6743 ± 0.0008
50,000	29.16	0.0542 ± 0.0002	0.6692 ± 0.0008	0.7234 ± 0.0009

According to table 4.2 the Inter Dancoff factor increases at first for increasing TRISO packing fractions, but reduces when the TRISO packing fraction is further increased. It was previously mentioned that increasing the number of TRISO particles or the TRISO packing fraction reduces

the amount of neutrons escaping the pebble. This should also reduce the Inter Dancoff factor. For low TRISO packing fractions there is however a chance that a neutron entering the fuel zone of another pebble will go through without crossing any fuel kernel. This chance decreases for increasing TRISO packing fractions. At first this effect dominates, resulting in a higher Inter Dancoff factor. Then for higher TRISO packing fractions and numbers of TRISO particles the reducing amount of neutrons escaping the pebble takes over and decreases the Inter Dancoff factor again. The Intra Dancoff factor dominates the total Dancoff factor. Since the Intra Dancoff factor increases for increasing TRISO packing fractions, the total Dancoff factor will increase as well, although less. The Dancoff factors from table 4.2 confirm these thoughts.

4.1.2 Wallpaper pebbles

Wallpaper fuel is a concept that has not been investigated much, despite the favourable temperature characteristics [7]. The influence of adding a central fuel free zone of various sizes on the Dancoff factor is studied here. To this end, Dancoff factors are calculated using MCDancoff-PB for different amounts of TRISO particles. This is done for both regular pebbles and wallpaper pebbles with a central fuel free zone of two different radii. The input parameters from table 3.1 are used. The results are shown in table 4.3.

Table 4.3: Intra, Inter and total Dancoff factors for regular and wallpaper fuel calculated by MCDancoff-PB.

N_{TRISO}	R_{middle} (cm)	pf~(%)	C_{intra}	C_{inter}	C
10,000	0	5.83	0.2670 ± 0.0005	0.0642 ± 0.0003	0.3312 ± 0.0006
10,000	1.5	7.44	0.2644 ± 0.0005	0.0715 ± 0.0003	0.3359 ± 0.0006
10,000	2.0	11.95	0.2721 ± 0.0005	0.0796 ± 0.0003	0.3517 ± 0.0006
25,000	0	14.58	0.4905 ± 0.0007	0.0692 ± 0.0003	0.5597 ± 0.0007
25,000	1.5	18.60	0.4879 ± 0.0007	0.0774 ± 0.0003	0.5653 ± 0.0008
$25,\!000$	2.0	29.88	0.4943 ± 0.0007	0.0862 ± 0.0003	0.5805 ± 0.0008
40,000	0	23.33	0.6143 ± 0.0008	0.0600 ± 0.0002	0.6743 ± 0.0008
40,000	1.5	29.76	0.6133 ± 0.0008	0.0664 ± 0.0003	0.6797 ± 0.0008

In section 4.1.1 it was shown that for regular pebbles an increase in the TRISO packing fraction causes a higher Intra Dancoff factor. For wallpaper fuel, adding a central fuel free zone increases the TRISO packing fraction by reducing the fuel zone volume. The results from table 4.3 however suggest that for a central fuel free zone of 1.5 cm the Intra Dancoff factor decreases at first. When the fuel free zone radius is increased to 2.0 cm, the Intra Dancoff factor does increase compared to regular pebbles, although only a little. This can be partially understood by realising that even though most neutron path lengths between fuel kernels are decreased, some path lengths through the central fuel free zone are considerably increased. This increase is in the order of the neutron mean free path in graphite from table 3.1. These neutrons are likely to suffer a moderator interaction, thus negating the decrease in moderator interactions for the shorter neutron path lengths. Additionally, the lumping of the fuel kernels near the fuel zone boundary has a twofold effect on the Intra Dancoff factor. Since the fraction of the surface 'filled' by fuel kernels increases, fewer neutrons generated closer to the center will be able to penetrate this layer and escape the pebble. On the other hand, neutrons generated inside this layer are more likely to escape the pebble, since there are no more fuel kernels to stop them. As said in section 4.1.1 the Intra Dancoff factor will decrease for an increase in the amount of neutrons escaping the fuel zone. For pebbles containing 10,000 TRISO particles (a packing fraction of 5.83%) the Intra Dancoff factor is computed by MCDancoff-PB for a full range of central fuel free zone radii (R_{middle}) to study the behaviour more closely. The results are plotted in figure 4.1. Input parameters from table 3.1 are used.

Figure 4.1 shows that the Intra Dancoff factor does indeed decrease at first as a regular pebble is modified into a wallpaper pebble by adding a central fuel free zone, with a minimum at half



Figure 4.1: The Intra Dancoff factor as a function of the central fuel free zone radius for 10,000 TRISO particles.

the fuel zone radius. For larger radii the Intra Dancoff factor increases again, with a maximum as R_{middle} equals approximately 90% of the fuel zone radius. After this maximum the Intra Dancoff factor decreases for the last two points shown in figure 4.1. Larger central fuel free zone radii were not investigated due to the TRISO packing fraction rising above 32%. For the reasons behind the complete behaviour some explanations were already provided, but more research is necessary to understand the exact mechanics. An important conclusion is nonetheless that the Intra Dancoff factor for wallpaper fuel changes only a little compared to that for regular fuel. The same behaviour applies for larger amounts of TRISO particles, but the minimum and maximum move relatively closer due to smaller differences in the configuration for increasing TRISO packing fractions. This can already be observed in table 4.3, though the data is very limited. The global behaviour for increasing the TRISO packing fraction or number of TRISO particles while keeping the central fuel free zone radius constant is the same as for regular fuel, which was elaborately discussed in section 4.1.1.

The Inter Dancoff factor is higher for wallpaper fuel than for regular fuel for both central fuel free zone radii investigated in table 4.3. It is mainly influenced by the amount of neutrons escaping the pebble, as found in section 4.1.1. It was already said while discussing the Intra Dancoff factor that it is unclear whether this amount increases or decreases for wallpaper fuel. Neutrons that escape the pebble do however have a larger chance of entering a fuel kernel in an adjacent pebble for wallpaper fuel. TRISO particles are located closer to the outer shell of the fuel zone, decreasing the necessary neutron penetration depth to enter another fuel kernel. This decreases neutron path lengths and thus decreases the chance of any moderator collisions. On top of that, neutrons are less likely to pass through the next fuel zone since the fraction of the outer surface 'filled' by fuel kernels is increased. These two effects cause the Inter Dancoff factor to increase for wallpaper fuel as compared to regular fuel, as shown in figure 4.2. In this figure the Inter Dancoff factor is plotted as a function of the central fuel free zone radius as computed by MCDancoff-PB for 10,000

TRISO particles. Input parameters from table 3.1 are applied.



Figure 4.2: The Inter Dancoff factor as a function of the central fuel free zone radius for 10,000 TRISO particles.

Figure 4.2 suggests an exponential dependence of the Inter Dancoff factor to the central fuel free zone radius. Since the chance of moderator collisions is exponentially dependent of the neutron path length, the decrease of these path lengths will most likely be the dominant cause in the increase of the Inter Dancoff factor. A clear answer as to how the amount of neutrons escaping the pebble is affected remains unknown and requires more research. Comparable results are found for the higher TRISO packing fractions listed in table 4.3. The results for a fuel free zone radius of 1.5 cm show an increase in the Inter Dancoff factor from 10,000 to 25,000 TRISO particles, and a decrease for 40,000 TRISO particles. This global behaviour for increasing the TRISO packing fraction or number of TRISO particles while keeping the central fuel free zone radius constant is the same as for regular fuel, as discussed in section 4.1.1.

The total Dancoff factor is the sum of the Intra and Inter Dancoff factor according to equation 2.10. Table 4.3 shows an increase in the total Dancoff factor for wallpaper fuel compared to regular pebbles for both central fuel free zone radii considered. In figure 4.3 the total Dancoff factor for 10,000 TRISO particles as computed by MCDancoff-PB is shown as a function of the central fuel free zone radius. The input parameters from table 3.1 are used.

The total Dancoff factor in figure 4.3 decreases slightly at first due to the decrease in the Intra Dancoff factor. Before the Intra Dancoff factor is at a minimum the Inter Dancoff factor, which exponentially increases, already more than compensates the decrease and causes an increase in the total Dancoff factor. For larger central fuel free zone radii the total Dancoff factor increases fast due to the increase in both the Intra and Inter Dancoff factor, up to the maximal Intra Dancoff factor. At this maximum, the changes in the Intra and Inter Dancoff factor more or less cancel each other. MCDancoff-PB was only used for TRISO packing fractions up to 32%, as mentioned in section 3.1.1, so the behaviour has not been investigated beyond this point. It is expected that the Intra Dancoff factor will decrease quickly, a trend which can already be observed in figure



Figure 4.3: The total Dancoff factor as a function of the central fuel free zone radius for 10,000 TRISO particles.

4.1, also reducing the total Dancoff factor. The largest difference in the Dancoff factor between wallpaper fuel and regular fuel for this configuration is approximately 10%. This largest difference becomes smaller for higher TRISO packing fractions. The differences between the minimum and maximum in the Intra Dancoff factor for the higher packing fractions considered in table 4.3 is comparable. The relative difference is decreased, because the related Dancoff factors are larger for these configurations. For a fixed central fuel free zone radius, the total Dancoff factor shows identical changes to that for regular pebbles when increasing the TRISO packing fraction or number of TRISO particles, as discussed in section 4.1.1.

Marmier et al. [7] found a difference of approximately 40% in the total Dancoff factor for wallpaper fuel compared to regular fuel, using a central fuel free zone radius of 0.884 times the fuel zone radius. They generated pebbles containing 15,000 TRISO particles with a modified version of PEBDAN [18]. The reported difference of 40% is much larger than the difference of 10% found here. The reasons for this conflict are unclear, mainly because the modifications Marmier et al. made to PEBDAN in order to make it applicable to wallpaper fuel were not described.

4.1.3 Dummy pebbles

Dummy pebbles can have a positive effect on the neutronics in a pebble bed reactor by increasing the amount of moderator interactions. Adding dummy pebbles to a pebble bed increases the average path length through graphite of neutrons that escape the pebble they were generated in, causing a decrease in the Inter Dancoff factor. The extend of this decrease is investigated here. The Inter Dancoff factor as a function of the fraction of dummy pebbles present inside the pebble bed is computed by MCDancoff-PB for several amounts of TRISO particles in both regular and wallpaper pebbles. The input parameters from table 3.1 are used for all calculations. Figure 4.4 shows the results for regular pebbles containing 10,000 (a packing fraction of 5.83%) and 50,000 (a packing fraction of 29.16%) TRISO particles. Other numbers of TRISO particles in between were also studied and yield similar results, but are omitted.



Figure 4.4: The Inter Dancoff factor as a function of the fraction of dummy pebbles for regular pebbles.

The Inter Dancoff factor decreases linearly with increasing dummy fractions in figure 4.4. The Inter Dancoff factor for no dummy pebbles and an Inter Dancoff factor of 0 for only dummy pebbles were interpolated to find the Inter Dancoff factor as a linear function of the fraction of dummy pebbles. This is analogous to multiplying the Inter Dancoff factor by a correction factor based on the dummy fraction (df), denoting the fraction of normal pebbles:

$$C_{inter}^{dummy} = C_{inter}(1 - df) \tag{4.1}$$

This method is most useful in practice, when only the Dancoff factor for no dummy pebbles is known. The Inter Dancoff factor for half the pebble bed filled with dummy pebbles shows the largest error with the linear interpolation. The maximal error between data points and the linear interpolation found in all configurations is 5%.

A possible explanation for the linear relation can be found in the probability that a neutron crossing a dummy pebble enters a fuel kernel in another pebble. If this probability can be neglected, a linear relation is to be expected. The probability that a neutron escaping a pebble enters a dummy pebble equals the fraction of dummy pebbles in the pebble bed. Assuming that all these neutron paths result in a moderator collision reduces the Inter Dancoff factor by the same factor, yielding a linear relation between the Inter Dancoff factor and the fraction of dummy pebbles. The mean chord length for a sphere equals [14]:

$$\langle l \rangle = \frac{4}{3}R\tag{4.2}$$

Using the pebble radius of 3.0 cm this results in neutrons travelling on average 4.0 cm through a dummy pebble, if of course they cross one. Then the 0.5 cm of the pebble shell they minimally

have to traverse twice in order to first escape a pebble and later enter the fuel zone of another pebble is added. This results in a conservatively estimated average path length of 5.0 cm through graphite when crossing a dummy pebble. Equation 3.2 then yields a 87% chance of a moderator collision happening on this path. The remaining 13% chance for a neutron to enter the fuel zone of another pebble can not be neglected. Neutrons however also travel some distance through both the fuel zones and the path length through the pebble graphite shell is on average larger than 0.5 cm. On the other hand, neutrons travelling only a small distance through a dummy pebble are still likely to enter a fuel kernel in another pebble. The results however suggest that the actual probability is small enough for a linear trend. Deviations from this trend, such as the high Inter Dancoff factor for 50% dummy pebbles, can be contributed to the probability that neutrons traversing a dummy pebble still enter a fuel kernel in another pebble. More research is required to verify these thoughts.

The influence of dummy pebbles on the Inter Dancoff factor is also investigated for wallpaper pebbles. The Inter Dancoff factor for wallpaper fuel with a central fuel free zone radius of 2.0 cm is plotted as a function of the fraction of dummy pebbles in figure 4.5. This is done for both 10,000 (a packing fraction of 11.95%) and 25,000 (a packing fraction of 29.88%) TRISO particles per pebble. Other central fuel free zone radii and numbers of TRISO particles were also studied and yield similar results. These are again omitted.



Figure 4.5: The Inter Dancoff factor as a function of the fraction of dummy pebbles for wallpaper pebbles with a central fuel free zone radius of 2.0 cm.

In figure 4.5 the same trends are observed for wallpaper fuel as for regular fuel in figure 4.4. The Inter Dancoff factor decreases linearly with increasing fractions of dummy pebbles and the Inter Dancoff factor for half the pebble bed filled with dummy pebbles shows the largest error with the linear interpolation. The largest error found between data points and the linear interpolation is again 5%. In section 4.1.2 it was mentioned that neutron path lengths in the fuel zone are decreased for wallpaper pebbles. This increases the previously calculated probability of neutrons entering a fuel kernel in another pebble when traversing a dummy pebble. Again the results

suggest that the actual probability is small enough for a linear trend, even though it is larger for wallpaper pebbles than for regular pebbles.

Dummy pebbles only affect the Inter Dancoff factor. In section 4.1.1 it was pointed out that the Intra Dancoff factor dominates the total Dancoff factor. Therefore, approximating the influence of dummy pebbles on the Inter Dancoff factor as a linear relation causes only a small error in the total Dancoff factor. The relative contribution of the Inter Dancoff factor to the total Dancoff factor is largest for small TRISO packing fractions. This contribution is nearly 20% for the smallest TRISO packing fraction considered in table 4.2. A maximal deviation of 5% in the Inter Dancoff factor then causes a deviation of only 1% in the total Dancoff factor, in the most extreme case considered here. For most applications this will be accurate enough. Modification of existing codes using this approximation will be very simple. Moreover, the analytical formula proposed by Bende et al. [17] is easily modified in section 4.3 using equation 4.1.

4.2 MCDancoff-WBC

Both differences between MCDancoff-WBC and MCDancoff-PB are separately validated in order to judge the reliability of this alternate approach, as described in section 3.2. First the use of only a single pebble instead of a complete pebble bed configuration is defended, then the application of the white boundary condition along its outer surface is justified. Additionally, Dancoff factors computed by both codes are compared to check for discrepancies. Following the code validation, both ways mentioned in section 3.2 to handle dummy pebbles are evaluated more thoroughly. Finally the major advantage of MCDancoff-WBC is shown by measuring the computation time needed to calculate the Dancoff factor.

4.2.1 Single pebble instead of a complete pebble bed

It was already shown in section 3.1.4 that using only one unique set of TRISO coordinates inside the pebbles within a pebble bed yields satisfying results for the Dancoff factor. Analogous to this conclusion, it is plausible to assume that a single pebble with white boundary conditions will also suffice, purely judging the geometry involved and not yet considering the implications on the neutron flight paths. Moreover, neutrons in MCDancoff-PB are generated in the middle of the pebble bed, which is analogous to dictating infinite reactor dimensions as discussed in section 3.1.4. This extra condition prevents neutrons from leaking out of the pebble bed. This is consistent with the possibilities for neutrons in MCDancoff-WBC, where a neutron will never even leave the pebble. Both methods only allow for neutrons to either count for the Dancoff factor or suffer a moderator collision. These arguments give reason to believe that MCDancoff-WBC will yield comparable results to MCDancoff-PB, as will be shown in section 4.2.3.

4.2.2 White boundary condition

The white boundary condition along the pebble outer surface is based on the assumption that the neutron direction while entering a pebble obeys a cosine distribution. The angular distribution for neutrons entering and leaving pebbles was studied before by, among others, Kloosterman and Ougouag [18] and by Ouwendijk [25]. Kloosterman and Ougouag report that, while the neutron direction leaving the pebble fuelzone is reasonably cosine distributed, the direction while leaving the pebble graphite shell is much more forwardly peaked, thus not obeying a cosine distribution. Ouwendijk, however, found that the neutron direction entering the pebble graphite shell does obey a cosine distribution. Since the white boundary condition only influences the neutron direction when reflected back *into* the pebble, it can be reasonably assumed that this direction is indeed cosine distributed. Another factor of uncertainty yet remains, namely the fact that the neutron exit point and entry point on the pebble graphite shell coincide for white boundary conditions. Although some effect should definitely exist, the results from section 3.1.4 suggest that it is negligible. There, the Dancoff factor for a pebble bed built with only identical pebbles with

exactly the same orientation was found to agree with the Dancoff factor computed for a realistic randomized pebble bed. This also causes a certain correlation between neutron exit and entry point on the pebble graphite shell, but does not affect the Dancoff factor within the error margins. Likewise, the white boundary condition is thought to have no significant influence on the computed Dancoff factor.

Another cosine distribution was implemented by Bende et al. [17] on the pebble fuel zone boundary, as mentioned in section 3.2. Based on the findings of Kloosterman and Ougouag and of Ouwendijk this seems reasonable. On the other hand, from a physical point of view neutrons are expected to penetrate the pebble shell while preserving their direction. To investigate the difference between these two methods, the Dancoff factor for 10,000 TRISO particles within a regular pebble, causing a 5.83% packing fraction, was computed by MCDancoff-WBC with and without sampling the neutron direction on the pebble fuel zone boundary. The results are listed in table 4.4. The input parameters are listed in table 3.1.

Table 4.4: Dancoff factors calculated by MCDancoff-WBC with and without sampling the neutron direction on the pebble fuel zone boundary.

Scatter on fuel zone boundary	C_{intra}	C_{inter}	C
yes	0.2666 ± 0.0005	0.0624 ± 0.0002	0.3290 ± 0.0006
no	0.2666 ± 0.0005	0.0639 ± 0.0003	0.3305 ± 0.0006

Clearly the results are comparable, although the Inter Dancoff factors do not agree within the maximal difference allowed by equation 3.4. Results for other pebble bed configurations are comparable. This shows that implementing another cosine distribution on the pebble fuel zone boundary induces a small error into the Dancoff factor. The physically correct situation and most accurate solution of no neutron scattering on the pebble fuel zone boundary is used in MCDancoff-WBC.

4.2.3 Code validation

Both differences between MCDancoff-WBC and MCDancoff-PB, namely using only a single pebble and implementing a white boundary condition along its outer surface, are now validated. The correct functioning of the entire code will be confirmed here. To this end Dancoff factors computed for a low and a moderately high packing fraction (pf) of TRISO particles within regular pebbles are compared in table 4.5. The results are listed for both FORTRAN codes using the input parameters from table 3.1.

Table 4.5: Dancoff factors calculated by MCDancoff-PB and MCDancoff-WBC for a low and a moderately high TRISO packing fraction.

Method	Input		$\mathbf{Results}$		
	N _{TRISO}	pf~(%)	C_{intra}	C_{inter}	C
MCDancoff-PB	10,000	5.83	0.2670 ± 0.0005	0.0642 ± 0.0003	0.3312 ± 0.0006
MCDancoff-WBC	10,000	5.83	0.2666 ± 0.0005	0.0639 ± 0.0003	0.3305 ± 0.0006
MCDancoff-PB	50,000	29.16	0.6692 ± 0.0008	0.0542 ± 0.0002	0.7234 ± 0.0009
MCDancoff-WBC	50,000	29.16	0.6688 ± 0.0008	0.0541 ± 0.0002	0.7229 ± 0.0009

As expected the results are in very good agreement. Comparable results are found for different configurations, including wallpaper fuel. This confirms that MCDancoff-WBC indeed computes Dancoff factors correctly. Also it is now verified numerically that the steps taken by Bende et al. [17] in deriving their analytical formula for the Dancoff factor are indeed valid. Only the slight modifications in MCDancoff-WBC are different from their method, such as ignoring the helium coolant and not scattering neutrons on the pebble fuel zone boundary. These may induce a small error into the analytical results, as was mentioned in section 4.2.2.

4.2.4 Dummy pebbles

Two methods for incorporating dummy pebbles were discussed in section 3.2. The first method is expanding the pebble graphite shell with the volume represented by dummy pebbles, in line with propositions made by Bende et al. [17]. The second method randomly transforms the pebble into a dummy pebble as a neutron reflects from the white boundary. This is done with a probability proportional to the relative number of dummy pebbles present inside the pebble bed. Both procedures were tested in MCDancoff-WBC and the resulting Inter Dancoff factors are listed in table 4.6 for various dummy pebble fractions. Reference data computed by MCDancoff-PB is also shown. Equal Intra Dancoff factors, within the statistical fluctuations, were found for all cases considered, independent of the amount of dummy pebbles as expected. The calculations were done for regular pebbles containing 10,000 TRISO particles per pebble, indicating a 5.83% packing fraction, but other configurations yield similar results. Other input parameters can be found in table 3.1.

Table 4.6: Inter Dancoff factors calculated by MCDancoff-PB and MCDancoff-WBC for various dummy pebble fractions.

		C_{inter}		
	MCDancoff-PB	MCDancoff-WBC		
Dummy pebble fraction		Transformation	Shell expansion	
0	0.0642 ± 0.0003	0.0639 ± 0.0003	0.0639 ± 0.0003	
0.25	0.0493 ± 0.0002	0.0487 ± 0.0002	0.0391 ± 0.0002	
0.50	0.0345 ± 0.0002	0.0332 ± 0.0002	0.0189 ± 0.0001	
0.75	0.0159 ± 0.0001	0.0169 ± 0.0001	0.0048 ± 0.0001	

Table 4.6 shows that the Inter Dancoff factor for the transformation method is comparable to that of MCDancoff-PB, whereas the shell expansion method gives far too low results. The transformation method was expected to yield satisfying results, since this method is nearly identical to the method used to incorporate dummy pebbles in MCDancoff-PB. Failure of the shell expansion method however makes the analytical formula proposed by Bende et al. inapplicable to dummy pebbles. The shell expansion method properly increases neutron path lengths through the graphite shell from one pebble to another, but also creates neutron paths through the expanded graphite shell, missing the pebble completely. This results in more moderator interactions than intended and consequently a decrease in the Inter Dancoff factor. These unintended neutron paths are shown in figure 4.6. The finalized version of MCDancoff-WBC of course handles dummy pebbles using the transformation method. In section 4.3 the analytical formula proposed by Bende et al. is slightly modified using the linear relation from equation 4.1 to correctly handle dummy pebbles.

4.2.5 Computation time

The main advantage of creating MCDancoff-WBC for calculating Dancoff factors is the reduction in computation time. Using only a single pebble with white boundary conditions removes the necessity of creating a complete pebble bed configuration. Since the creation of unique sets of TRISO coordinates takes longer for increasing TRISO packing fractions, as already mentioned in section 3.1.1, this can make a large difference. The creation of a single set of TRISO coordinates increases from a few seconds for 10,000 TRISO particles (5.83% packing fraction) up to almost 2 hours for 50,000 TRISO particles (29.16% packing fraction), both for regular pebbles. In section 3.1.1 it was pointed out that these created sets of TRISO coordinates were written to files in order to save time for subsequent calculations. These sets therefore only have to be created once, reducing the advantage of MCDancoff-WBC as more calculations are performed.

The simulation of neutron flight paths within the helium coolant however requires a lot of computation time as well, since the distance to each pebble is calculated in this area. In MCDancoff-PB pebble beds containing up to 67,500 pebbles were generated, which indicates a lot of extra



Figure 4.6: Intended and unintended neutron paths for the shell expansion method.

computation time for each neutron escaping the first pebble. While reading in the sets of TRISO coordinates, in that manner eliminating the time needed to create those, Dancoff factors for regular pebbles were computed by both MCDancoff-PB and MCDancoff-WBC for a low and moderately high TRISO packing fraction (pf). The smallest pebble bed containing only 5,005 pebbles was used in MCDancoff-PB. Using the exact same input parameters in both codes, the computation time needed for the calculations is listed in table 4.7.

Table 4.7: Computation time for MCDancoff-PB and MCDancoff-WBC for a low and moderately high TRISO packing fraction while reading in the sets of TRISO coordinates.

Method	N_{TRISO}	pf~(%)	Computation time (hours)
MCDancoff-PB	10,000	5.83	1.0
MCDancoff-WBC	$10,\!000$	5.83	0.25
MCDancoff-PB	50,000	29.16	2.0
MCDancoff-WBC	$50,\!000$	29.16	0.50

Both results in table 4.7 indicate a factor *four* decrease in computation time while using MCDancoff-WBC. It is however strange that the relative decrease in computation time for both TRISO packing fractions is the same. Only neutrons escaping the first pebble should cause a decrease in computation time for MCDancoff-WBC compared to MCDancoff-PB. This amount of neutrons is roughly the same for both TRISO packing fractions, or even smaller for the higher packing fraction as mentioned in section 4.1.1. The absolute difference in computation time should therefore be approximately the same for both packing fractions. The results here could be influenced by differences between the cores on which the calculations were performed or other tasks being performed on the same core. Nevertheless, the improvement in computation time is

significant, especially when considering that only 5,005 pebbles were generated in MCDancoff-PB. The computation time reached here might even make it worthwhile to separately compute Dancoff factors and subsequently use them as input for criticality calculations when a high accuracy is required. All calculations were performed on the hpc11 cluster at the Reactor Institute Delft.

4.3 The modified analytical formula

The analytical formula proposed by Bende et al. [17] from equation 2.13 can be easily modified using the linear dependence of the Inter Dancoff factor to the dummy fraction from equation 4.1. The Dancoff factor then becomes:

$$C = C_{\infty}^{fk} \left[1 - P_F \left(\Sigma^* R_{fuelzone} \right) + C_{\infty}^{FZ} (1 - df) \frac{P_F \left(\Sigma^* R_{fuelzone} \right) \left[1 - T_{II} \right]}{1 - T_{II} T_{IO} T_{OI}} \right]$$
(4.3)

Kloosterman and Ougouag [18] found that the analytical formula calculates Dancoff factors with an accuracy of approximately 2%. In table 3.5 it was shown that MCDancoff-PB yields Dancoff factors of approximately 2% higher than the analytical formula for a low TRISO packing fraction. For such a low TRISO packing fraction, the linear approximation for dummy pebbles also induces the largest error to the Dancoff factor, as was shown in section 4.1.3. This error may be as much as 1% of the Dancoff factor. Considering these errors, the final error in the modified analytical formula may be as much as 3% for small TRISO packing fractions. These thoughts are verified by the Dancoff factors for a low and moderately high TRISO packing fraction in table 4.8, calculated using MCDancoff-PB and the modified analytical formula. Results calculated using the orignal analytical formula while expanding the graphite shell are also shown to emphasise the improvement gained with the modification. The input parameters from table 3.1 and a dummy fraction of 0.50, inducing the largest error when using the linear approximation, are applied.

Table 4.8: Dancoff factors calculated by MCDancoff-PB, the modified analytical formula and the original analytical formula for a low and a moderately high TRISO packing fraction and a dummy fraction of 0.50.

Method	Input		Results			
	N_{TRISO}	pf~(%)	C_{intra}	C_{inter}	C	
MCDancoff-PB	10,000	5.83	0.2670 ± 0.0005	0.0345 ± 0.0002	0.3015 ± 0.0005	
Modified formula	10,000	5.83	0.2625	0.0306	0.2931~(-2.79%)	
Original formula	10,000	5.83	0.2625	0.0175	$0.2800 \ (-7.13\%)$	
MCDancoff-PB	50,000	29.16	0.6692 ± 0.0008	0.0294 ± 0.0002	0.6986 ± 0.0008	
Modified formula	50,000	29.16	0.6738	0.0256	$0.6994 \ (+0.11\%)$	
Original formula	50,000	29.16	0.6738	0.0152	0.6890 (-1.37%)	

Since the Dancoff factor is underestimated by the analytical formula for low TRISO packing fractions and the linear approximation for dummy pebbles also underestimates the Dancoff factor, the total error in the modified analytical formula is largest for low TRISO packing fractions. It is approximately 3% when compared to MCDancoff-PB in table 4.8, as expected. As a comparison, the total error for the shell expansion method in the original analytical formula is as high as 7%, more than twice as much. For high TRISO packing fractions, the analytical formula slightly overestimates the Dancoff factor. Therefore the error in the modified analytical formula is reduced due to the underestimation of the Dancoff factor in the linear approximation for dummy pebbles. This is also shown in table 4.8. The shell expansion method again yields much worse results.

The modified analytical formula is a very fast method for calculating Dancoff factors. The influence of the Dancoff factor on the multiplication factor as described in section 2.2, which was tested by Kim et al. [19], suggests that the reached accuracy may induce an error of approximately 1% in k_{eff} . If this accuracy is sufficient, the modified analytical formula is preferable over time-consuming numerical methods. It is certainly preferable over the original analytical formula, due

to at least twice as small errors when dummy pebbles are introduced. It however remains desirable to find a means of calculating the Dancoff factor analytically with a higher accuracy, both with and without dummy pebbles, to fully replace numerical methods.

Chapter 5 Conclusions and recommendations

The main goal of this research was to numerically calculate Dancoff factors in pebble bed reactors as a function of various design parameters, specifically for wallpaper fuel and dummy pebbles. To this end MCDancoff-PB was created, a code to calculate Dancoff factors in a fully generated pebble bed. Using MCDancoff-PB, the dependence of the Dancoff factor to the TRISO packing fraction, number of TRISO particles and the fuel zone radius was investigated for regular pebbles. The difference between regular fuel and wallpaper fuel was then studied for a full range of central fuel free zone radii in the wallpaper design. Finally, the influence of dummy pebbles on the Dancoff factor was determined. Furthermore, a second code called MCDancoff-WBC was developed to numerically verify the steps taken by Bende et al. [17] in deriving their analytical formula. This code also provides a less time-consuming method of numerically evaluating Dancoff factors. Using results for dummy pebbles the analytical formula proposed by Bende et al. was also modified to be applicable to pebble bed configurations containing dummy pebbles within reasonable accuracy. The conclusions of the studies conducted in this research are summarised in section 5.1, followed by recommendations for future work in section 5.2.

5.1 Conclusions

Using MCDancoff-PB, the Dancoff factor in regular pebbles was found to be dominated by the TRISO packing fraction. For increasing TRISO packing fractions, the Intra Dancoff factor also increases due to the reduction of neutron path lengths in the moderator and the reduction in the amount of neutrons escaping the fuel zone. The number of TRISO particles a pebble contains is relevant as well, because higher numbers reduce the amount of neutrons escaping the fuel zone, increasing the Intra Dancoff factor. Finally, the fuel zone radius is important to control the TRISO packing fraction according to equation 3.1. The Inter Dancoff factor was found to increase at first for increasing TRISO packing fractions, due to the higher probability of entering a fuel kernel in another pebble. For even higher TRISO packing fractions it was found to reduce again, due to the reduction in neutrons escaping the pebble fuel zone. The total Dancoff factor is dominated by the Intra Dancoff factor and therefore increases for increasing TRISO packing fractions and numbers of TRISO particles.

The Dancoff factor for wallpaper fuel follows the same trends as the Dancoff factor for regular fuel when varying the TRISO packing fraction by changing the fuel zone radius. When varying the central fuel free zone radius for a constant fuel zone radius however, the results are surprising. The Intra Dancoff factor was shown to decrease when increasing the central fuel free zone radius up to half the fuel zone radius, and to increase for larger central fuel free zone radii up to 0.9 times the fuel zone radius. After this maximum it decreases again, although it was not studied for TRISO packing fractions higher than 32%. Reasons for this behaviour remain unclear, since there are explanations for both an increase and a reduction in the Intra Dancoff factor. The TRISO packing fraction increases when increasing the central fuel free zone radius, thus reducing neutron path lengths through the moderator. On the other hand, some neutron path lengths that go through the central fuel free zone are drastically increased. Due to the lumping of fuel kernels near the fuel zone outer shell, neutrons are prevented from escaping the pebble fuel zone. Neutrons generated in this lump are however more likely to escape since they are closer to the outer shell. The Inter Dancoff factor increases for an increase in the central fuel free zone radius due to this fuel lumping near the fuel zone outer shell. The observed dependence was exponential, suggesting this increase is caused by a reduction in moderator interactions and thus path lengths. The total Dancoff factor decreases only slightly for a small central fuel free zone radius and increases significantly for larger central fuel free zones. The maximal difference measured between the Dancoff factors for regular fuel and wallpaper fuel was 10%. This means that the Dancoff factor for wallpaper fuel may be approximated by that for regular fuel, especially for small central fuel free zone radii.

The Inter Dancoff factor was found to be linearly affected by the fraction of dummy pebbles present inside the pebble bed. The Inter Dancoff factor for any dummy fraction can therefore be approximated by the Inter Dancoff factor without dummy pebbles, multiplied by the fraction of normal pebbles, as shown in equation 4.1. A possible explanation is the small probability that neutrons traversing a dummy pebble will still enter a fuel kernel in another pebble, although this can not be the only explanation. The linear approximation underestimates the Inter Dancoff factor by a maximum of 5% for a dummy fraction of 0.5. Considering the measured maximal contribution of 20% of the Inter Dancoff factor to the total Dancoff factor, the induced error in the total Dancoff factor is approximately 1%. This can be sufficient for many purposes, providing an easy and fast method of dealing with dummy pebbles.

MCDancoff-WBC was used to validate the steps taken by Bende et al. [17] in deriving their analytical formula. It generates only a single pebble and incorporates a white boundary condition along its outer surface. Only the implementation of a cosine distribution on the pebble fuel zone boundary was found to be slightly inaccurate. MCDancoff-WBC was observed to produce accurate Dancoff factors when compared to MCDancoff-PB without implementing this extra cosine distribution. The use of only a single pebble and a white boundary condition along its outer surface very well approximates a complete pebble bed. Moreover, a factor four decrease in computation time was measured for MCDancoff-WBC when compared to MCDancoff-PB. These results are however not in line with physical expectations. Additional uncertainties may have been present and should be identified. Adding up the volume of dummy pebbles to regular pebbles, thus accounting for the increase in neutron path lengths through the moderator, was found to produce inaccurate results. Instead transforming the pebble to a dummy pebble upon a white boundary reflection did yield satisfying results, reducing the error in the total Dancoff factor by at least a factor 2 when compared to the shell expansion method.

The analytical formula proposed by Bende et al. [17] was slightly modified by multiplying the Inter Dancoff factor with the fraction of normal pebbles to be applicable to pebble bed configurations containing dummy pebbles. This modified formula allows for the calculation of Dancoff factors within an accuracy of approximately 3%. This induces an uncertainty of approximately 1% in the multiplication factor, when compared to the results of Kim et al. [19]. For applications in which this uncertainty suffices, the modified formula is a very fast method of calculating Dancoff factors. It was found to yield results at least twice as accurate as the original analytical formula when dummy pebbles were present.

5.2 Recommendations

Dancoff factors calculated in this research were made independent of the pebble bed dimensions. Moreover, the TRISO coating layers were homogeneously mixed with the graphite matrix. Finally, the graphite cross section was held constant, even though it is a function of the neutron energy as mentioned in section 2.1.1. These approximations allow for the study of the influence of other parameters to the Dancoff factor more closely. They are however certainly relevant when designing a pebble bed reactor and should be accounted for. It should be verified that the observed behaviour still exists for a physically correct situation. The Dancoff factor found for wallpaper pebbles shows surprising behaviour. The exact mechanisms behind this behaviour are unknown. More research should be conducted to investigate how many neutrons travel through the central fuel free zone, how many of these suffer moderator collisions, and how many neutrons manage to escape the pebble to explain the results found here. Furthermore, it would be interesting to study the behaviour of the Dancoff factor for very large central fuel free zone radii, which were omitted here because the TRISO packing fraction then exceeds 32%.

The Dancoff factor was found to linearly depend on the fraction of dummy pebbles. Exactly why this linear relation occurs is still unknown. It was suggested that this relation is related to the probability that a neutron traversing a dummy pebble enters a fuel kernel in another pebble. This probability should be investigated, as well as other causes for the results found here.

MCDancoff-WBC was shown to require less computation time to calculate Dancoff factors than MCDancoff-PB. The observed difference in computation time was however not in line with the expectations. The simulations should be redone to verify the results and eventual causes of uncertainty should be identified.

The analytical formula proposed by Bende et al. [17] was modified to be applicable to pebble bed configurations containing dummy pebbles. The resulting error in the Dancoff factor of approximately 3% is however still large for certain applications. More research should be conducted to find an analytical formula that yields results accurate enough to replace numerical methods, thus drastically reducing the time needed to calculate the Dancoff factor for any desired pebble bed configuration.

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