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Serpent 2 simulations of the historic Haigerloch B8 nuclear reactor of 1945

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Abstract: We use Serpent 2 as a contemporary Monte Carlo tool to simulate the effective neutron multiplication factor k_{eff} of the historic Haigerloch B8 nuclear reactor designed by Heisenberg and Wirtz in February to April 1945. The device parameters are either measured in the Haigerloch replica, taken from the historic reports or adapted from literature. We obtain k_{eff} = 0.952 which coincides with previously calculated results reported in the literature, but which is larger than the historically reported measured value of k_{eff} = 0.85. In addition, we tune the design parameters in order to reveal the most important device characteristics. We find an optimized reactor set-up that, under the condition to use as little uranium and heavy water as possible, is characterized by an increase of the vessel diameter by 35 % which would have brought the reactor to criticality with the available amount of uranium fuel. We show that the bottleneck would have been the lack of a sufficient amount of heavy water which would have been almost two-and-a-half times the then available quantity to reach criticality.

Keywords: nuclear reactor kinetics; criticality; history of science; Monte Carlo simulations

MSC: 82D75; 81V35

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1 Introduction

1.1 Historical background

The Italian Enrico Fermi tried to create new artificial (transuranic) elements by bombarding uranium with slow neutrons. When repeating the experiments in Berlin in December 1938, Otto Hahn and Fritz Strassmann discovered nuclear fission, while Lise Meitner, being Jewish, who had to flee from Nazi Germany from Berlin to Sweden in July 1938, provided the theoretical calculations and the explanation of the unstable uranium nucleus after the capture of an additional neutron. Already four months later, Paul Harteck, the director of the Institute of Physical Chemistry at the Universität Hamburg, and his assistant Wilhelm Groth wrote a letter dated April 24, 1939 to the Heereswaffenamt (German Army Ordnance Office). They alerted the military of a potential of a chain reaction and the principle possibility of an "explosive". The Army Ordnance Office in the Reich Ministry of War was in the Third Reich responsible for the development of new weapons. Several publications on the potential practical application of the nuclear fission arrived there in the sequel. Another four months later in August 1939, Siegfried Flügge wrote a public newspaper article in the Deutsche Allgemeine Zeitung entitled with "The utilization of nuclear energy" (orig. "Die Ausnutzung der Atomenergie"). Directly afterwards, Dr. Kurt Diebner, physicist and the person in charge in the German Army Ordnance Office, invited to the first Uranium Conference in Berlin on September 16, 1939. The "uranium club" was founded.

The result of this first uranium conference was that all measures for clearly answering the question of the technical feasibility of nuclear energy production should be taken. Werner Heisenberg should first work out the theory of the nuclear reactor. During a follow-up conference in October 1939, Heisenberg was asked whether it would be possible with the discovery of Otto Hahn to produce nuclear weapons. Heisenberg basically answered that from the physics point of view, it would be conceivable, but the technical and economic problems he rated as serious enough that a production of the bomb would not be possible within the next few years. After the conferences, the experimental work aiming at the construction of a nuclear reactor (called uranium machine) was distributed over different locations, where different geometrical arrangements of the set-up were realized and tested.

At the Universität Leipzig, the sequence L1 to L4 of experiments was realized by Werner Heisenberg and Robert Döpel (Heisenberg and Wirtz 1947). They used a spherical arrangement of fuel and heavy water as a moderator. A positive neutron multiplicity could be achieved for the first time with the experiment L4 in June 1942, indicating the realization of a short-time chain reaction. A similar experiment was realized in parallel by Fermi in Chicago only a few weeks later. During the same month, a reactor exploded in Leipzig because of an unexpected chemical reaction of uranium metal with water. Kurt Diebner was the first to use an array of uranium cubes in the sequence G1 to G3 at the Army Research Center in Berlin-Gottow. This brought improved results as compared to the arrangement with uranium plates used before that (Heisenberg and Wirtz 1947).

In the Kaiser-Wilhelm-Institute of Physics (KWI) in Berlin-Dahlem, Werner Heisenberg, Karl Wirtz, Carl-Friedrich von Weizsäcker realized the series B1 to B7 of experiments (Heisenberg and Wirtz 1947). The KWI worked with uranium plates and heavy water as a moderator. Due to air strikes in Berlin, the research work was transferred to a small town in the South-West of Germany. The institute was moved to Hechingen, while an experimental research site was started in a small cave in the town of Haigerloch located a few kilometers away from Hechingen. A former beer cellar was rented by the Kaiser-Wilhelm-Gesellschaft and the experimental set-up started in late 1944. Together with Fritz Bopp and Emil Fischer, the last experiment B8 was realized in April 1945. After the transfer from Berlin, this group then also used an arrangement with uranium cubes as suggested by Diebner for the first time.

The transfer from Berlin to Hechingen and Haigerloch was initiated by Walter Gerlach, in charge of nuclear physics at the Reichsforschungsrat (German Research Council) acting under the Ministry of Armaments and War Production. He had been appointed successor of his Ph.D. advisor Friedrich Paschen in 1925 as a professor of physics at the Universität Tübingen (Hagmann 2023), about 40 km away from Haigerloch. During his time in Tübingen, Gerlach probably traveled the surroundings, thereby visiting the idylic town of Haigerloch situated in a narrow limestone valley, such that it could be safe from air attacks.

In this work, we re-address the historic Haigerloch nuclear reactor experiment B8 from the point of view of modern simulation tools of neutron dynamics. As is known, it never reached criticality, but the measured neutron multiplicity reached a maximum value of $M = 6.7$ of all experiments carried out during World War II in Nazi Germany. The B8 reactor was realized as a cylindric device, with an outer vessel placed in a concrete pit in the floor of an underground cave which had been used as a beer cellar in Haigerloch. The outer vessel contained a layer of graphite blocks used as a neutron reflector. Inside, an inner cylinder vessel was placed that contained heavy water as the moderator. The fuel was shaped in the form of cubes that hang from the lid of the closed vessel along aluminum wires. An external neutron source was inserted through a central chimney. In addition, radially placed chimneys were used to insert glass tubes as measurement probes. The major advancement compared to the previous experiments until B8 was the use of a regular arrangement of the uranium fuel in the form of cubes of natural uranium metal, suspended in the inner vessel.

1.2 Modern simulation techniques applied to the historic B8 reactor

Modern numerical simulation techniques, especially those based on the Monte Carlo method, have nowadays reached a high level of maturity and are routinely being applied in the design of modern nuclear reactors. Back in the 1940s of the last century, scientists could only dream of such tools. It is therefore quite appealing to analyze historical reactor concepts in view of present knowledge and understanding using such modern tools. The Haigerloch B8 reactor has been studied by numerical techniques before. Grasso et al. (2009) reported results for k_{eff} and M, its neutron energy-distribution spectrum, and its neutron-flux distribution in its central horizontal and vertical planes for both thermal and fast neutrons using the Monte Carlo neutron transport code MCNP5 (Sweezy et al. 2003). It is a general-purpose, continuous-energy, generalized-geometry, time-dependent, coupled neutron-photon-electron Monte Carlo transport code that was developed at Los Alamos National Laboratory. It is a widely used tool for designing and analyzing nuclear reactors and is an alternative to Serpent 2. Grasso et al. (2009) estimated $k_{\mathrm{eff}} = 0.86$ based on a simplifying assumption that the uranium-fuel cubes and the aluminum-wire links are treated as a kind of homogenized material, in the sense that they could be modeled as effective cylinders of a phenomenological diameter. The cylinders were assumed to be filled with a uniform and homogeneous mixture of uranium fuel, aluminum, and heavy water, with the materials placed inside each cylinder.

Pešić (2018) used a more accurate modelling of the geometry and a follow-up version MCNP6.1 of the Monte Carlo neutron transport code with the latest ACE type neutron nuclear cross section data at that time. A careful description of essential geometrical details of the arrangement of the uranium cubes and the wire suspensions together with updated material parameters yielded a much larger effective neutron multiplication factor of $k_{\mathrm{eff}} = 0.953$. In addition, Pešić (2018) could study many different detailed variants of the reactor configurations, taking into account the unknown geometric details or material configurations (alloys, purities, contaminations, etc.).

Park (2022) reported improved MCNP simulations. He used the precise form of the uranium cubes and their historically reported arrangement. In addition, he referred to recent mass spectroscopy measurements of the density of an original uranium cube at the Pacific NW National Lab (PNNL). The measured value amounts to 18.53 g/cm^3, which has to be compared by the nominal magnitude of 19.05 g/cm^3 of natural uranium as used in the present work and by Pešić (2018). Furthermore, Park (2022) used a historically determined purity of the heavy water obtained in a measurement in 1947 of the Haigerloch heavy water kept at NIST. By this, Park (2022) further refined the value to $k_{\mathrm{eff}} = 0.958$ in his analysis of the Haigerloch reactor.

1.3 Outline of the present study

In this study we use the contemporary Monte Carlo tool Serpent 2 (Leppänen et al. 2015) to perform simulations of the B8 experiment and to calculate the criticality parameters. We emphasize especially on building a model in Serpent 2 that reconstructs the historical design and material composition of the B8 experiment as close as possible, using data from either historic reports, from recent measured data at the Atomkeller Museum Haigerloch, Germany, or from literature. We therefore present first our best estimate of the design of the Haigerloch B8 reactor as well as of the properties of the used materials. We then compare the results of the effective neutron multiplication factor from our Serpent 2 simulations with the historically reported value of Heisenberg and Wirtz (1947) as well as the results reported from previous work (see above). We find that the historic configuration realized in the B8 experiment is rather close to the optimum given the circumstances of limited resources and equipment. In addition, we have varied key reactor parameters in the simulations in order to understand which of the parameters have a major impact on criticality. We investigate the enrichment of uranium and also analysed the effect of the unknown degree of contamination of the heavy water with light water and with boron. Furthermore, we conducted a systematic parametric study to evaluate the impact of the fuel element spacing on the effective neutron multiplication factor k_{eff}. While keeping the total volume of heavy water constant, we adjusted the geometry of the core accordingly in order to maintain consistent moderation conditions. Finally, we answer the question by what decent modifications of the reactor set-up under the historic circumstances criticality would have been reachable.

2 The design of the Haigerloch B8 reactor

Determining the dimensions of the original historic Haigerloch reactor is challenging, since the original device was destroyed in 1945 and the historic documentation remained incomplete. A careful discussion of this issue is given in the work by Pešić (2018). Here, we use a combination of three approaches: (1) parameters reported in the original historic report of Heisenberg and Wirtz (1947), (2) parameters measured in the replica model (present state May 2024) in Haigerloch, and (3) parameters rationalized in Pešić (2018). A sketch of the B8 set-up is shown in Figure 1. The replica model is considered credible due to its reconstruction being guided by historical photographs, surviving documentation, and input from individuals familiar with the original reactor. Historic documentation is available and is shown in Figure 2. The left panel shows a sketch of the device, while the right panel depicts the reproduction of an original photograph of the device of 1945. Photographs of the contemporary replica model are shown in Figure 3.

2.1 Concrete cylinder

The reactor as a whole was embedded in a pit in the floor of the Atomkeller cave in Haigerloch. For this, a cylindrically shaped concrete wall and a concrete floor were designed in which the reactor was inserted and which eventually served as a (normal) water pool. The diameter of the original concrete construction was measured in Haigerloch to be 300.0 ± 0.2 cm (Würth WDM 30 laser rangefinder) and the height of the concrete cylinder has been measured as 254.1 ± 0.2 cm.

2.2 Uranium cubes and their suspension

The fuel consisted of cubes of natural uranium with a edge length of 5 × 5 × 5 cm. In agreement with the historic reports, the replica of the device also contained replica cubes (of aluminum) in the same size. In addition, one original uranium cube is still conserved up to present in the Haigerloch

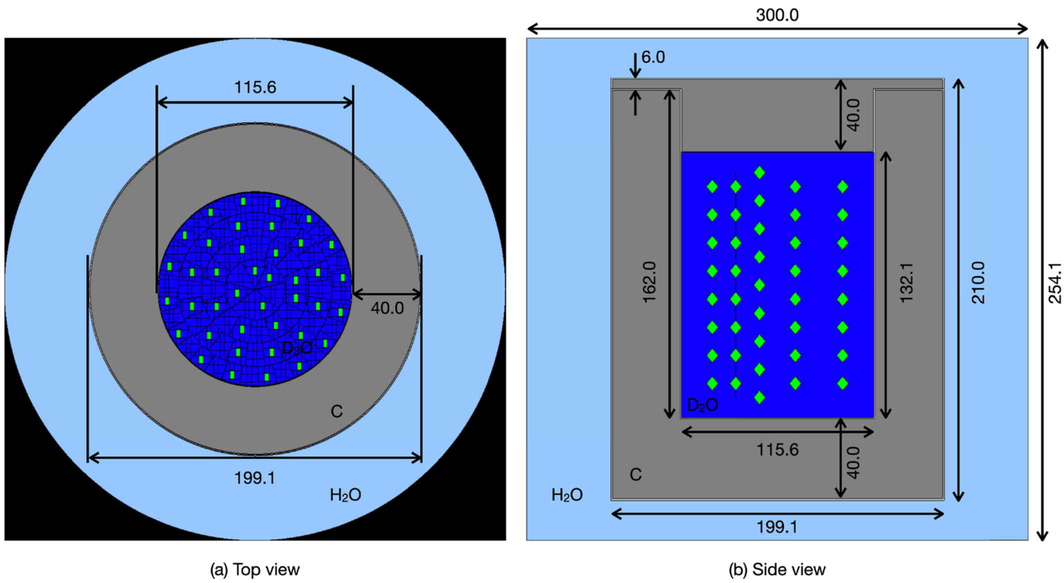

Figure 1: Serpent 2 plot of the historic Haigerloch B8 reactor, (a) top view and (b) side view. The green symbols represent the uranium cubes, which are connected by aluminum cables (black thin lines, barely visible). The dark blue region indicates the heavy water inside the magnesium tank, which is surrounded by the graphite reflector (dark grey). The light blue area corresponds to the light water. Not all cubes are visible, as the plots includes sectional (horizontal and vertical) planes. The wall thicknesses of the aluminum and magnesium tanks are not visible on this scale. The chains of the uranium cubes are arranged regularly as described in the text. The top lid includes as well a lower magnesium part, a graphite layer and a covering aluminum top part. The dimensions are given in units of cm. The wall thicknesses of the vessels are not shown.

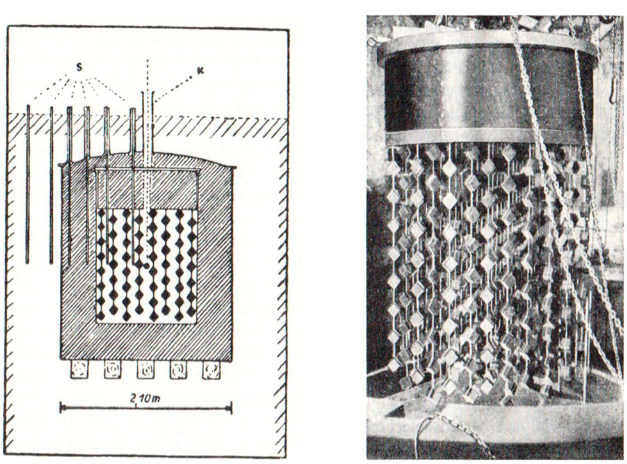

Figure 2: Left: Scheme of the experiment B8 (reproduced from Heisenberg and Wirtz (1947)) with the neutron source placed in the center, the uranium cubes with the aluminum wires, the graphite reflector (hatched area). The vessel is placed on wooden supports. S indicates six probing tubes placed radially from the center. The central tube marks the chimney used to insert the neutron source and to insert the heavy water. Right: original photograph of the B8 reactor (reproduced from Heisenberg and Wirtz (1947)).

Figure 3: Contemporary photographs of the replica reactor reconstructed at the Atomkeller Museum Haigerloch taken in May 2024 by the authors. Left: inner vessels of the reconstruction. Right: top part with the replica of the uranium cubes.

Atomkeller museum. From previous experiments, Heisenberg realized that an optimal cube edge length would be 6–7 cm (Heisenberg and Wirtz 1947). Since a larger amount of cubes with edge length of 5 cm were left over from the Gottow experiments, those cubes were used and complemented by further produced cubes of 5 cm edge length (Heisenberg and Wirtz 1947).

The uranium cubes themselves were not clad, but coated with a polystyrene emulsion to protect them from chemical reactions with air or water and to minimize radiation exposure for the operators (Grasso et al. 2009), but this was not taken into consideration in the simulation. 664 cubes were arranged vertically in a chain along aluminum wires such that the (end-to-end) distance between the cubes amounts to an average value in the replica of 6.85 cm. To obtain this value, we measured the distance between several randomly sampled cubes in the replica. This is consistent with the reported center-to-center distance of the cubes of 12 cm. In total, there are 40 chains carrying nine uranium cubes and 38 chains carrying eight cubes. The 78 chains are arranged in alternating order in four concentric rings (counted from the outside inwards with 32 chains in the outermost ring, and then 23 chains, 15 chains, and eight chains (innermost ring). The diameter of the aluminum suspension wire forming the chain was measured in the replica at four different random samples, yielding a mean value of 3.35 ± 0.05 mm (Caliper). In the historic report, Heisenberg and Wirtz (1947) note that neither the cube dimensions nor their distances were optimal, but had to be taken as given due to the general circumstances in early 1945.

2.3 Reactor core and inner magnesium vessel

The dimensions of the reactor core cylinder vessel have been measured at the replica. We have found an inner diameter of the magnesium cylinder of 115.6 ± 0.20 cm (Würth WDM 30 laser rangefinder) and have used this in the simulations. The number slightly deviates from the number reported by Heisenberg and Wirtz (1947) which is 124 cm. The total height of the magnesium cylinder is 162.0 ± 0.20 cm. This magnitude is in decent agreement with the historic one reported as 164 cm (Heisenberg and Wirtz 1947). We have measured a wall thickness of the replica of 0.368 ± 0.005 cm (Caliper) which also coincides with the magnitude of the wall thickness of 0.3 cm reported by Heisenberg and Wirtz (1947).

2.4 Graphite reflector

The thickness of the graphite layer as the reflector is well documented (Heisenberg and Wirtz 1947). We use a layer thickness of 40.0 cm at the cylinder walls and at the bottom of the cylinder. We note that the replica in the museum shows a graphite layer thickness of 30.6 cm, which does not correspond to the value published in the original historic report. The thickness of the graphite layer in the lid is in reality slightly larger, but for simplicity, we use the same value of 40.0 cm also for the lid (the replica in the museum is somewhat irregular due to construction and yields a value of 47.8 cm which we believe is not realistic). Furthermore, the graphite had been used in the form of rectangular blocks with the dimension 5 × 10 × 50 cm (Heisenberg and Wirtz 1947) and arranged in the cylinder layer. Due to these circumstances, small gaps filled with air remained, but are considered as irrelevant for the present analysis.

2.5 Aluminum outer vessel

The wall thickness of the aluminum tank could be measured directly at the original device which is still conserved at the Haigerloch museum as the only original piece. It has been destroyed by explosives in May 1945 and left back by the military ALSOS mission. Despite being strongly deformed, its wall thickness can still be measured. We have measured the wall thickness of the outer aluminum vessel as 0.783 ± 0.005 cm (Caliper). This value slightly deviates from the number of 0.5 cm reported by Heisenberg and Wirtz (1947). We believe that this difference is of minor relevance.

Due to the disagreement of the thickness of the graphite layer between the published value and the value measured at the replica, we believe that the value of the diameter of the outer aluminum tank of the replica in the museum is not reliable. Instead, we have calculated the inner diameter of the aluminum tank according to twice the wall thickness plus twice the graphite layer thickness plus the diameter of the magnesium core cylinder. We find 199.1 cm for the diameter of the outer aluminum tank. This value is also slightly in disagreement with the number of 210 cm for the diameter reported by Heisenberg and Wirtz (1947).

The height of the aluminum outer tank is taken from the literature as 210 cm, which is consistent with the sum of the height of the magnesium cylinder and twice the thickness of the graphite layer (one in the bottom and one in the lid) which amounts to 212 cm.

2.6 Neglected components and simplifications

In order to simplify the Serpent 2 simulations, we neglect the metal enforcement construction inside the top part of the reactor which carries the suspended chains with the uranium cubes. The enforcement construction needed to be used in order to carry the total weight of the suspended uranium cubes of about 1.5 tons. Then, we use a planar geometry of the lid of the aluminum vessel and neglect the vault present in the original form designed for mechanical stability reasons. Furthermore, we did not take into account the fact that the uranium cubes were suspended in an intertwined pair of aluminum wires, but used only one wire in the simulations. In addition, we did not include the wooden bars at the bottom of the concrete pit on which the outer aluminum vessel was placed. Finally, we did not take into account the gaps in the inner vessel and the graphite reflector used in the original construction to insert six cylindrically shaped tubes of the neutron detecting probes. Likewise, the chimney in the center of the lid which was used to insert the initial neutron source and to gradually fill the heavy water into the inner vessel is not part of the arrangement used in the simulations. In agreement with Pešić (2018), we believe that these simplications are adequate and do not affect the overall result in a substantial manner. The geometrical parameters of the reactor components used in the simulations are summarized in Table 1 and can also be visually traced in the schematic representation shown in Figure 1.

3 Properties of the materials used in the Haigerloch B8 reactor

Some of the material parameters involved have been reported by Heisenberg and Wirtz (1947). However, following Pešić (2018), the composition of the materials in the reactor could only be reconstructed and there are some uncertainties in the historical data. Therefore, the precise composition of the materials and their contamination with others is estimated based on sources and historical circumstances, or different variants are assumed. We use the material parameters compiled by Pešić (2018), which are summarized below and in Table 2.

Table 1: Approximate dimensions of the historic B8 reactor. The values given are based on literature references, measurements taken on the reactor replica or well-founded estimates. Differences are due to rounding errors.

Component	Diameter (cm)	Height (cm)	Wall thickness (cm)
Concrete cylinder	300.0	254.1	–
Reactor core cylinder	115.6	132.1	–
Mg tank	116.3	162.0	0.4
Graphite reflector (outer ring)	–	210.0	40.0
Graphite reflector (bottom)	199.1	40.0	–
Graphite reflector (lid)	199.1	40.0	–
Al tank	200.7	210.0	0.8
Reactor lid	199.1	6.0	–
Reactor lid insert	115.6	34.0	–

Table 2: Material compositions of the Haigerloch B8 reactor as used in this work and by Pešić (2018) and as used by Grasso et al. (2009).

Material	This work and Pešić (2018)		Grasso et al. (2009)	
	Density	Composition	Density	Composition
Natural uranium (nUm)	19.05 $\frac{g}{cm^3}$	Impurities: 1–20 ppm EBC, typically 5 ppm	19.05 $\frac{g}{cm^3}$	Not specified
Heavy water (D_2O)	1.11 $\frac{g}{cm^3}$	95 % D_2O, 5 % H_2O	1.11 $\frac{g}{cm^3}$	95 % D_2O, 5 % H_2O
Aluminum alloy 1100 (outer vessel)	2.71 $\frac{g}{cm^3}$	Al: min. 99.0 %, Fe: max. 0.95 %, Si: max. 0.95 % (combined with Fe), Cu: 0.05–0.20 %, Zn: max. 0.10 %, Mn: max. 0.05 %, Others: max. 0.05 % each, 0.15 % total	2.71 $\frac{g}{cm^3}$	Al: 99.0 %, Fe: 0.4 %, Si: 0.5 %, Cu: 0.08 %, Zn: 0.15 %
Aluminum alloy 5025 (wire)	2.64 $\frac{g}{cm^3}$	Al: 95.0 %, Mg: 5.0 %	2.64 $\frac{g}{cm^3}$	Al: 95.25 %, Mg: 3.9 %, Si: 0.25 %, Fe: 0.2 %, Zn: 0.2 %, Cr: 0.15 %, Cu: 0.04 %, Mn: 0.01 %
Magnesium alloy AZ91 (inner vessel)	1.83 $\frac{g}{cm^3}$	Mg: approx. 90 %, Al: 8.5–9.5 %, Zn: 0.5–1.0 %	1.83 $\frac{g}{cm^3}$	Mg: 90.2 %, Al: 8.0 %, Zn: 1.0 %, Si: 0.5 %, Cu: 0.1 %, Mn: 0.13 %, Ni: 0.07 %
Graphite	1.7 $\frac{g}{cm^3}$	Pure graphite, lower density due to block arrangement	1.8 $\frac{g}{cm^3}$	C: 99.925 %, remainder: see Table 3 in Grasso et al. (2009)

3.1 Natural uranium

The fuel consisted of the form of natural metallic uranium (nUm) that has a typical density of 19.05 g/cm^3 and contained impurities measured as the equivalent boron content (EBC). The EBC value varied between 1 ppm and 20 ppm, with 5 ppm EBC assumed as the average (Pešić 2018).

3.2 Heavy water D_2O

D_2O was used as a moderator. Values of 95 % D_2O and 5 % H_2O were used for the reference calculation of the nominal design. However, due to historical uncertainty, the purity of the heavy water is varied between 89 % and 99 % D_2O in the sensitivity calculations. The density and atomic density are determined at a temperature of 293.15 K (Pešić 2018).

3.3 Aluminum alloy 1100

Aluminum alloy 1100, also known as Al 1100, is a commercially pure aluminum alloy with an aluminum content of at least 99.0 %. A density of 2.71 g/cm^3 is specified in this work (Alloys International Inc. 2024). It is characterised by excellent corrosion resistance, good formability and high thermal and electrical conductivity. This alloy is frequently used in heat exchangers, chemical equipment and food processing equipment. In the Haigerloch B8 reactor, it was used as the material for the outer aluminum vessel (Pešić 2018). The composition of Al 1100 includes (United Aluminum 2024): aluminum (Al): min. 99.0 %, iron (Fe): max. 0.95 %, silicon (Si): max. 0.95 % (combined with iron), copper (Cu): 0.05–0.20 %, zinc (Zn): max. 0.10 %, manganese (Mn): max. 0.05 %, other elements (each): max. 0.05 %, and other elements (total): max. 0.15 %.

3.4 Aluminum alloy 5025

For the suspension of the uranium cubes in the reactor core, wires made of aluminum alloy 5025 was used (Pešić 2018), which consists of 95 % aluminum and 5 % magnesium (Aluminum Association 2024). The density is given as 2.64 g/cm^3. This alloy offers a good mix of mechanical strength and malleability.

3.5 Magnesium alloy AZ91

In the Haigerloch B8 reactor, AZ91 magnesium alloy was used for the inner magnesium vessel (Pešić 2018). This alloy is widely used and consists mainly of magnesium (approximately 90 %), aluminum (8.5–9.5 %) and zinc (0.5–1.0 %) (Magnesium Elektron 2024). A density of 1.83 g/cm^3 is specified in the source. It is known for its excellent castability, high strength and good corrosion resistance. It is frequently used in the automotive industry, for electronic housings and in the aerospace industry.

3.6 Graphite

For the reflector material, a detailed analysis of the graphite used is difficult. A detailed discussion is presented by Pešić (2018). Different types of graphite were used in the reactor (Pešić 2018). Pure graphite has excellent neutron moderating properties, while graphite with 1 ppm EBC corresponds to nuclear-grade graphite, which has low impurities and is therefore ideal for nuclear applications (Pešić 2018). Natural graphite has an impurity density of 4.212 ppm EBC. This graphite contains natural impurities that can slightly affect its moderation properties (Pešić 2018). Eventually, we have used pure graphite (or, graphitic carbon) with a density of 1.7 g/cm^3, as described by Heisenberg and Wirtz (1947). We did not explicitly account for certain air gaps between the prebuilt graphite blocks used. They have emerged due to the geometric arrangement of the blocks in the outer wall of the reactor.

4 Simulation approach

As mentioned above, we use in this study the computer code Serpent 2 (Leppänen et al. 2015) to perform simulations of the B8 experiment. Serpent 2 simulates a large number of stochastic neutron trajectories in complex reactor geometries based on the Monte Carlo method. Initially, the spatial and spectral distribution of the neutron source (i.e. the neutrons generated essentially by the fisson of U-235 nuclei) is unknown. Therefore, Serpent 2 has to generate an initial guess for the first generation of neutrons at the start of the simulation. The positions, direction vectors and energies of the neutrons are determined randomly. The initial positions are sampled either uniformly or from distributions representing typical spatial flux distributions in reactors, such as Bessel and cosine function shapes for the radial and vertical direction. The direction vectors are also being randomly selected, with a preference towards their source, as well as the energies of the neutrons distributions that depend on the specific source of the neutrons, such as fission or an external neutron source. The calculation of a neutron trajectory is performed by means of a sequence of discrete steps. Doing this, the calculation has to take into account the geometrical distribution and the physical properties of the materials in the reactor through which the neutron propagates. These properties depend on the density (number) and require specific nuclear data for all of the isotopes of which the different materials (fuel, moderators, supporting structures etc.) are composed. These nuclear data are available in the form of libraries, such as e.g. the Joint Evaluated Fission and Fusion (JEFF) Library or the ENDF/B Evaluated Nuclear Data Library. They provide the cross sections, i.e. probability distributions, of neutron-induced interactions (e.g. capture, fission, scattering) as well as further probability distributions, e.g. for decay data, fission yields, and neutron activation. The libraries use different native formats to store the data, which can be converted to the ACE ('A Compact Evaluated Nuclear Data File') format which is used by the Serpent 2 code. At the beginning of a step, the current state of a neutron is known either from inital conditions or from the previous step. In order to determine the state at the end of the step, first the new position of the neutron is determined, using the known direction vector and the path length of the step which is determined by drawing a random sample from the distribution characterized by the total cross section for neutron interactions. The calculation of the path length is a non-trivial task, because during one step the neutron may cross regions with different material properties, i.e. the cross sections used to draw the sample for the path length are not valid for part of the path. Therefore, Serpent 2 uses a special method called "Delta tracking" (Leppänen et al. 2015) to increase numerical efficiency by introducing virtual collisions to skip the explicit calculation at cell boundaries with changing material parameters. After the new position along the trajectory is known, the type of neutron-induced interaction is determined randomly, taking into account the probabilities of the potential interactions (which depend on the energy of the neutron and material properties at the new position). In case of a capture or a fission reaction, the trajectory of the neutron is terminated. If a fission reaction took place, the number of new neutrons as well as their direction and energy are determined randomly based on respective probability distributions. These properties, together with the position of the fission, are stored to form the source for the next generation of neutrons. Otherwise (i.e. in the case of scattering), the energy and the direction of the neutron are updated, and the calculation proceeds to the next step of the trajectory. Within one generation, the trajectories of all neutrons are followed until these are either terminated by a capture/fission reaction or are lost by leaving the domain over the boundaries. Then, by averaging over all trajectories in one generation, the effective neutron multiplication factor k_{eff} can be calculated, together with an estimate of the statistical uncertainty. Because the initial distribution of source neutrons can only be guessed, it will in general deviate from the distribution of source neutrons resulting from following the trajectories of all neutrons of a generation (and memorizing the new neutrons created by fission). The fact, that the neutron source distribution varies from generation to generation implies that also the effective neutron multiplication factor k_{eff} varies accordingly. Thus, an iterative procedure is required, which involves calculating a sequence of neutron generations until the difference between the effective neutron multiplication factors k_{eff} of two subsequent generations is deemed sufficiently small to conclude on convergence.

5 Results of the reference case using best estimate parameters

For the reference case we have used the best estimate parameters described above to determine the criticality of the Haigerloch reactor B8 using Serpent 2. Further, we used the Joint Evaluated Fission and Fusion (JEFF) Library version 3.1.1 for the nuclear data. The scattering kinematics and scattering cross sections of bound nuclides are additionally affected by the chemical bonds at thermal energies, which can have an important effect especially on the thermal scattering for the light and heavy water as well as the graphite. Since this is not considered in the standard JEFF library, we additionally activated in Serpent 2 the option to take into account the temperature dependence of bound-atom scattering according to the $S(\alpha, \beta)$ law available from the ENDF80SaB2 Thermal Scattering Data library. Moreover, we have used the Serpent run parameters *set pop 5000 60 20* and *set bc 1*. The boundary conditions have been set to open boundary conditions (1 = vacuum), which is typical for closed reactor models.

For the conditions of the reference case the effective neutron multiplication factor was obtained as

$$k_{\text{eff}} = 0.9517 \pm 0.00048. \tag{1}$$

In the historical documents the neutron multiplicity M has been used instead of k_{eff}. The two factors are related by

$$M = \frac{1}{1 - k_{\text{eff}}}. \tag{2}$$

The effective neutron multiplication factor k_{eff} represents the average number of neutrons produced in a single fission-chain generation by one parent neutron. After n fission generations, the number of neutrons per initial neutron is k_{eff}^n. Therefore, the total number of neutrons M in the fission chain per starting neutron amounts to $M = 1 + k_{\text{eff}} + k_{\text{eff}}^2 + k_{\text{eff}}^3 + \ldots$. This is a geometric series that converges to $1/(1 - k_{\text{eff}})$ for values of $k_{\text{eff}} < 1$. For a critical or supercritical reactor with $k_{\text{eff}} \geq 1$, the series diverges and M becomes infinite. M is therefore not a suitable variable for expressing criticality across the entire possible spectrum, in contrast to k_{eff}. In order to evaluate the uncertainty due to cross section data, the calculation was repeated using the nuclear library ENDFb71 instead of JEFF 3.1.1. With otherwise unchanged data we obtain $k_{\text{eff}} = 0.9499 \pm 0.00101$, i.e. the relative difference of 0.0019 is of the order of magnitude of the statistical error. Further, we investigated the effect of neglecting the temperature dependence of bound-atom scattering, using both JEFF 3.1.1 and ENDFb71 libraries.

With JEFF 3.1.1 we find k_{eff} = 0.9502 ± 0.00052 and with ENDFb71 k_{eff} = 0.9539 ± 0.00098. Again, these are relative differences in the order of the statistical error.

The result obtained in the present work matches fairly well with those of recent studies. Pešić (2018) reported k_{eff} = 0.953 and Park (2022) reported k_{eff} = 0.958. These two authors used the MCNP-6 code instead of Serpent 2, but otherwise followed a quite similar approach as in the present study, in particular by modeling the precise form of the uranium cubes and their historically reported geometrical arrangement. Differences between the work of Pešić (2018) and ours mostly concern slightly different geometric extensions. Park (2022), in addition, used a slightly different density of the uranium fuel which he determined from extant cubes in a measurement at the Pacific NW National Lab (PNNL) by mass spectroscopy. The measured value amounts to 18.53 g/cm^3, which has to be compared by the nominal magnitude of 19.05 g/cm^3 of natural uranium as used in the present work and by Pešić (2018). Further, referring to a measurement from 1947 of an original sample of the Haigerloch heavy water kept at NIST, Park (2022) assumed a higher D_2O purity of 96.8 % instead of the 95 % used by Pešić (2018) and us.

Compared to the recent studies, Grasso et al. (2009) yielded a significantly lower result for the effective neutron multiplication factor of k_{eff} = 0.86. Grasso et al. also used the neutron transport code MCNP, however the previous version 5 with respective cross section libraries. The main difference to the more recent studies is the simplified modeling of the fuel elements in the work of Grasso et al. Instead of modeling the geometry of the uranium cubes and the aluminum suspensions explicitly, each column of hanging cubes was replaced by an equivalent cylinder. Each cylinder contained eight or nine fuel cubes, the aluminum wires and a proportionate amount of the heavy water. These materials were assumed to be homogeneously mixed within the cylinders, which had an equivalent diameter of $10/3\sqrt{6}$ cm. Usually, the homogenization of the fuel and structural materials results in a reduced accuracy of the neutron flux distribution and reactivity estimates.

Heisenberg and Wirtz (1947) reported a neutron mutiplication factor of M = 6.7 which results in k_{eff} = 0.85. It remains unclear why the coinciding results of Pešić (2018), Park (2022) and ours do not match the historically reported value of Heisenberg and Wirtz. From the results on the basis of slightly different choices of the parameters in the three works mentioned, we can conclude that the final results of the critically are quite insensitive to the small variations. Possible reasons for the deviations remain speculation. One possible reason could be that the purity of the graphite and/or of the heavy water used in the Haigerloch B8 reactor was substantially lower than assumed in the modern simulations. Another possible reason could be that the procedure of measuring the neutron production used in 1945 had some unknown shortcomings. In early 1991, a motion picture entitled “Das Ende der Unschuld” was shot in the Haigerloch museum. As a scientific advisor, Erich Bagge, a former member of the ‘Uranverein’ was present. He described the measurement procedure which was afterwards reenacted in the movie. Glass tubes with dysprosium oxide disolved in nitric acid were inserted in five vertical tubes with increasing radial distance to the reactor axis (Heisenberg and Wirtz 1947). The dysprosium solution was activated until saturation. Then, the glass cylinders were removed from the reactor and the dysprosium solution was passed in front of a Geiger-Müller counter in order to count the activity. Further details on this measurement procedure are not documented. In view of the significant deviations between the modern calculated magnitudes and the historically reported magnitude of k_{eff}, it remains unclear how reliable this measurement procedure was. Further, the nuclide Dy-164 that was activated to Dy-165 to measure the neutron flux is a strong neutron absorber. As mentioned in Section 2, the tubes with the dysprosium solution have not been included into the model in previous and also not in the present study. This should be taken into account by future work.

In the present work, the neutron multiplication factor was calculated in each case under the assumption that the materials are at room temperature. However, the configurations assumed in the calculations can in reality only be reached by a relatively slow transient process (e.g. in the Haigerloch B8 experiments the heavy water was filled slowly and stepwise into the inner vessel), during which the materials would start to heat up due to the thermal power from nuclear fission. This would lead, due to the negative reactivity coefficients of fuel and moderator temperature and, if applicable, the void coefficient to significantly smaller values of the neutron multiplication factor than those calculated for the “cold” state. However, such a more realistic determination of criticality would require coupled transient simulations of neutronics and thermohydraulics. The effort required for this would go beyond the scope of the present investigations. In the present analyses the focus is on comparing the potential criticality of different geometric and material configurations. For this purpose, we consider the simplified calculation without consideration of thermal effects to be sufficient, although the results at least for the cases with neutron multiplication factors significantly larger than 1 have to be considered as fictitious.

6 Variations in the reactor design

In this section, we investigate the impact of possible variations of the parameters used in the simulations. These include modifications of the geometry of the fuel arrangement and the form of the fuel as well as an increased enrichment of the uranium. In addition, the choice of the reflector material and its dimension have an impact. We simulate the use of beryllium as reflector material and different wall thicknesses of the reflector. In addition, a crucial quantity is the contamination of the heavy water with light water or boron. Finally, we address the question of a mere scale-up of the total dimension of the reactor in order to achieve criticality.

6.1 Effect of fuel arrangement: variation of uranium cube size and distance

It is well known that the criticality of a reactor depends strongly on the geometrical arrangement of the fuel and the moderator, since this has, together with thermal effects, an important impact on moderation and capture/fission probabilities. In general, increasing the size of a fuel element increases the probabilities for fissions but also for parasitic captures by non-fissile material. Increasing the space between the fuel elements (filled with moderator) improves the thermalization of the neutrons and thus the probability of fissions, but also increases the risk of captures (e.g. due to impurities). Thus, there should exist optimum values or ranges for the fuel element dimensions and spacing. As mentioned above, already, Heisenberg and Wirtz (1947) noted that a larger size of the fuel cubes with an edge length between 6 and 7 cm should be optimal for criticality. However, due to practical reasons (5 cm cubes left over from the Gottow experiments), the edge length of the cubes of the historical B8 reactor was chosen as 5 cm. Also, their distance in both horizontal and vertical directions of 14 cm was rather determined by the available amount of heavy water than by optimality criteria. In modern days, the parameters of the geometrical arrangement of the core region can be easily varied in simulations in order to study the effect on the criticality. This was also done by Pešić (2018), though he used specifically for his parametric calculations on the fuel element size and the spacing a simplified model. This was comprised only of a representative fuel cube within a cube filled with heavy water (of varying purity) with an edge length corresponding to the quadratic pitch between elements. Selective boundary conditions were applied for this representative fuel cell, i.e. he determined the effective neutron multiplication factor k_{inf} while neglecting the escape of neutrons. In our study, we used the reactor model to perform parametric calculations with variations of the geometrical configuration in the core. Doing so, of course unrealistic configurations, e.g. when the edge length of the cube exceeds the distance between the cubes, or, the cube becomes too small in relation to the distance, as would be the case for an edge length of 1 cm and a distance of 20 cm, were omitted in our simulations. The results are given in Table 3 and shown in Figure 4.

In addition, in Figure 4, k_{eff} is plotted as a function of the edge length of the cubes for three different horizontal distances between the cubes. The diagram shows that k_{eff} is largest for a distance of 10 cm for a cube edge length of ≤4 cm. Since the cubes in this configuration are small

Table 3: Dependence of k_{eff} on the edge length of a cube as well as the horizontal and vertical distances between the cubes.

Edge [cm]	$x-y$-spacing (cm)	z-Spacing (cm)	k_{eff}
1	10	10	0.1374 ± 0.00071
1	14	14	0.0936 ± 0.00039
2	10	10	0.5269 ± 0.00073
2	14	14	0.3765 ± 0.00085
2	20	20	0.1478 ± 0.00062
3	10	10	0.7937 ± 0.00116
3	14	14	0.6743 ± 0.00085
3	20	20	0.3169 ± 0.00095
4	10	10	0.8859 ± 0.00091
4	14	14	0.8504 ± 0.00089
4	20	20	0.4951 ± 0.00110
5	10	10	0.8677 ± 0.00101
5	14	14	0.9517 ± 0.00048
5	20	20	0.6498 ± 0.00102
6	10	10	0.7896 ± 0.00102
6	14	14	0.9536 ± 0.00099
6	20	20	0.7424 ± 0.00102
7	10	10	0.7052 ± 0.00081
7	14	14	0.9224 ± 0.00092
7	20	20	0.8584 ± 0.00090
8	10	10	0.6448 ± 0.00177
8	14	14	0.8629 ± 0.00102
8	20	20	0.9073 ± 0.00098
10	10	10	0.5942 ± 0.00177
10	14	14	0.6849 ± 0.00091
10	20	20	0.9276 ± 0.00097
12	14	14	0.5536 ± 0.00107
12	20	20	0.8695 ± 0.00101
14	20	20	0.7639 ± 0.00094

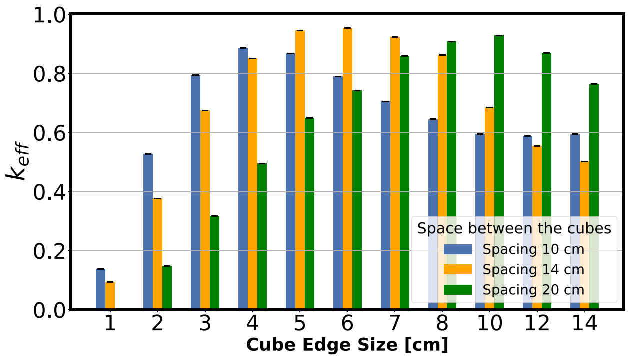

Figure 4: k_{eff} as a function of the edge length in cm of the cubes for three different horizontal distances between the cubes of 10 cm, 14 cm and 20 cm as indicated.

compared to the distance, this is an expected result, as the neutrons are less likely to reach the nearest uranium atom outside the cube at larger distances. For an edge length of 5–7 cm, the distance between the cubes of 14 cm is optimal. For an edge length of 8 cm, the distance of 20 cm yields the maximum effective neutron multiplication factor.

Our results obtained with the Serpent 2 code are largely consistent with those of Pešić (2018), who used the MCNP code and concluded, that the optimum edge length should be 6–7 cm. Figure 4 shows that in our calculations the maximum effective neutron mulitplication factor arises for edge lengths of the uranium cubes in the range of 5–8 cm. However, in Pešić's results k_{eff} reached values up to 1.3 (with a lattice pitch of 20 cm and pure heavy water) using the simplified fuel cell model, while according to our results increasing the edge length and the pitch is not sufficient to make the reactor critical.

To summarize, there are two configurations with a significant maximum, namely with an edge length of 6 cm and a distance of 14 cm, and an edge length of 10 cm and a distance of 20 cm. The advantage when increasing the edge length of the cubes is due to the larger amount of fuel. However, larger cubes also require larger distances because a sufficient amount of moderator is needed to induce criticality. It should also be kept in mind that a larger distance must lead to an enlargement of the reactor, which consequently also requires more heavy water. However, a larger edge length also means a larger demand of uranium, which was difficult to obtain in 1945. Since an edge length of 5 cm at a distance of 14 cm produces a result similar as for the other edge lengths, an edge length of 5 cm at a distance of 14 cm is the optimal solution in view of the scarcity of fuel and moderator materials, if the cubic shape of the fuel is utilized. It is a remarkable result that Heisenberg hit the optimal reactor design in 1945 by analytical calculations, without access to nowadays simulation tools.

6.2 Effect of fuel geometry: uranium spheres and cylinders

In this section, we examine the question of whether a different form of the fuel element would have led to a large effective neutron multiplication factor under certain conditions. As an alternative to cubes, we examine spheres and cylinders. In order to be comparable with the previous arrangement, the mass (resp. the volume) of the fuel should be kept constant. Determining the diameter of a sphere that has the same volume as a cube with edge length of 5 cm yields a diameter of 6.2 cm. Using the spheres instead of the cubes while keeping all other parameters identical to the reference case (see Section 5), we find $k_{\text{eff}} = 0.9511 \pm 0.00043$.

Next, we investigate the effect of the spatial arrangement of the fuel spheres by reducing the distances between the spheres. This has the effect that the “core region”, i.e. the region filled with dispersed fuel elements becomes smaller, i.e. the fuel is more concentrated in a smaller part of the reactor. This has, firstly, the effect that the fuel-to-moderator ratio increases and, secondly, that the lateral or vertical water colums acting as reflectors become thicker. The results for k_{eff} depending on different spacings between fuel elements are given in Table 4. We find that a reduction in the distances in the z- or x-direction between the uranium spheres leads to a smaller effective neutron multiplication factor.

A reduction in the size of the spheres and the associated reduction in spacing could lead to an improvement in the effective neutron multiplication factor, while the amount of uranium used should remain the same, meaning that more spheres would have to be suspended. However, the suspension of the spheres poses a challenge, as this is difficult to realize for smaller sphere diameters. In addition, the fuel-to-moderator ratio should be kept optimal and there should remain enough amount of moderator between the fuel spheres.

Table 4: Dependence of k_{eff} on the distances between uranium spheres.

Sphere diameter	Distance in z	Distance in x and y	k_{eff}
6.2 cm	14 cm	14 cm	0.9511 ± 0.00043
6.2 cm	10 cm	14 cm	0.9358 ± 0.00063
6.2 cm	14 cm	10 cm	0.9220 ± 0.00047

Another option would have been to arrange the fuel in the form of cylinders, similar to the fuel rods of nowadays light water reactors. Here, we investigate the effect of the shape of the fuel element in a simplified way and neglect the necessity of suspending the fuel e.g. by stacking uranium pellets inside a clad tube. To ensure that the same amount of uranium is used as in the reactor with uranium cubes, an equivalent diameter of the cylinders has to be determined. It is assumed that each column of cubes suspended by the same wire is replaced by one cylinder and that the uranium cylinders have the same height as the entire reactor core. Equating the total volume of the uranium cubes with the total volume of the cylinders and solving for the diameter gives approximately 3 cm. For simplicity, we keep the horizontal distance from one cylinder to the next at 14 cm. All other geometries of the original B8 reactor are kept unchanged. By this, we obtain $k_{eff} = 0.9420 \pm 0.00074$.

To further investigate this configuration, we varied the cylinder diameter and the horizontal spacing. The parameter "inner circle" refers to the radial distance from the reactor center to the first ring of concentric fuel wires, as used in the original B8 setup. Reducing the inner circle from its original value of 11 cm leads to a higher concentration of fuel near the center and reduces the amount of moderator available in the core region. This has a similar effect to the reduction of the core region discussed for the spherical configuration in Table 4, where a smaller fuel zone increases the fuel-to-moderator ratio and thickens the outer reflector, but also reduces moderation inside the core. The results are given in Table 5.

We find that the lateral distance between the cylinders and their diameter have a significant influence on the effective neutron multiplication factor. An optimum is achieved with larger distances, such as for 14 cm and 15 cm, as shown in Table 5. This is due to the increasing amount of moderator present for increasing the distance between the cylinders. Furthermore, another optimum is found for a cylinder diameter of 5 cm and a distance of 14 cm, where $k_{eff} = 0.9500 \pm 0.00074$ is achieved which is merely due to the increased amount of fuel. Compared to the calculated effective neutron multiplication factor of the reactor with uranium cubes of 5 cm edge length and a distance of 14 cm in all directions of $k_{eff} = 0.9517 \pm 0.00048$, the magnitude for the cylinder configuration with a diameter of 3 cm and a distance of 14 cm yields $k_{eff} = 0.9420 \pm 0.00074$, which shows that the choice of cubes, under fixed parameters, is better.

We find that the lateral distance between the cylinders has a significant influence on the effective neutron multiplication factor. An optimum is achieved with larger distances, such as for 14 cm and 15 cm, as shown in Table 5. This is due to the increasing amount of moderator present when increasing the distance between the cylinders. Compared to the calculated effective neutron multiplication factor of the reactor with uranium cubes of 5 cm edge length and a distance of 14 cm in all directions of $k_{eff} = 0.9517 \pm 0.00048$, the configuration with cylindrical fuel elements of 3 cm diameter and the same 14 cm spacing results in $k_{eff} = 0.9420 \pm 0.00074$, which shows that the choice of cubes, under fixed parameters, is slightly more favourable.

Yet, the spherical and especially cylindrical geometry of the fuel could have been an alternative option to obtain a critical reactor. However, this would have required extensive modifications to the historical reactor design.

Table 5: Tuning the diameter of the uranium cylinders for different horizontal (*x*- and *y*-direction of the cylinders). By this, the diameter of the inner circles arises as indicated on the condition that the total amount of fuel remains unchanged as compared to the historic experiment.

Cylinder diameter	Horizontal center-to-center spacing	Radius of first fuel inner ring	k_{eff}
3 cm	5 cm	5 cm	0.6732 ± 0.00083
3 cm	5 cm	11 cm	0.7880 ± 0.00095
3 cm	10 cm	11 cm	0.9259 ± 0.00072
3 cm	14 cm	11 cm	0.9420 ± 0.00074
3 cm	15 cm	10 cm	0.9400 ± 0.00069
3 cm	20 cm	10 cm	0.8597 ± 0.00087

6.3 Effect of fuel enrichment

The potential of enrichment of the isotope U-235 has been early recognized by the German scientists. However, the technical challenges of implementing the project on the required scale were considered too great and the focus was laid on reaching criticality with natural uranium and heavy water only. From a nowadays perspective is nevertheless interesting, which degree of enrichment would have been sufficient to make the B8 reactor in Haigerloch critical. For this purpose we carried out parametric calculations using enriched uranium oxide of different degrees of enrichment. The enrichment stages are based on the stages used by the NEA and are enrichment of UOX levels from 0.7 % to 4.55 %.

Figure 5 shows that the effective neutron mulitiplication factor strongly increases with enrichment, as expected. The reactor would have been supercritical already with an enrichment of 1 % leading to a $k_{eff} = 1.0062 \pm 0.00036$.

However, in this configuration the reactivity $\rho = (k_{eff} - 1)/k_{eff}$, which measures the departure from criticality, has a value of 0.0062, while the fraction of delayed neutrons according to the Serpent 2 results is $\beta_{eff} = 0.00712$, i.e. the reactor

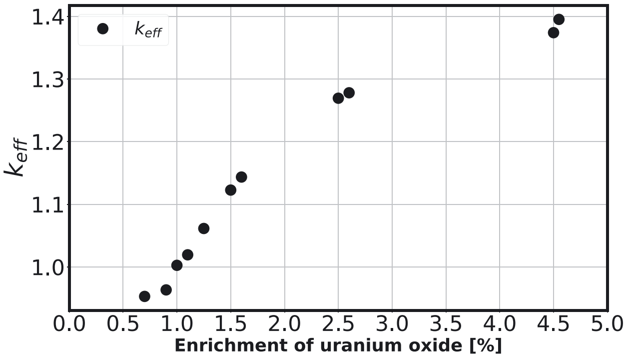

Figure 5: k_{eff} of the Haigerloch B8 reactor as a function of the enrichment of uranium. The left-most data point marks natural uranium which was used in the historical set-up.

would already have been dangerously close to prompt supercriticality. If the reactivity ρ exceeds the fraction of delayed neutrons β_{eff}, the neutron flux and therefore the power increases exponentially due to the prompt neutrons alone. The corresponding time constant is then determined by the average lifetime of the free neutrons, which is of the order of magnitude of 1 ms in a moderated reactor (instead of the time constant of a delayed critical reactor, which is in the order of magnitude of seconds). This extremely rapid increase leads to an uncontrolled power excursion, as it can no longer be influenced quickly enough by external technical means.

The designers of the B8 reactor were well aware of the risk of an uncontrolled power excursion and had foreseen respective countermeasures. Heisenberg's concept realized this in the form of cadmium rods (Heisenberg and Wirtz 1947), which could have been introduced via the chimneys on the upper side of the reactor, as can be seen in Figure 2. The experiment in Haigerloch proceeded by gradually filling in the heavy water into the reactor core and constantly monitoring the neutron multiplicity. In this sense, prompt supercriticality would have been rather unlikely, since the experiment could have been stopped in the case of a significantly rising multiplicity. In this sense, the experiment B8 was a "critical experiment" in modern language since modern approaches to reactor control typically involve measuring k_{eff} in the subcritical state with a neutron source to safely approach criticality. Since the neutron multiplicity is proportional to $1/(1 - k_{\text{eff}})$, the reciprocal of the neutron detector reading is plotted against the level of the heavy water inside the reactor core.

In passing, we note that the mentioned criticality can only be achieved with the historically original geometries and materials. The heavy water has a particularly large influence here. If the heavy water in the reactor core was to be replaced by light water, a much smaller magnitude of $k_{\text{eff}} = 0.3439 \pm 0.00072$ would result, even with an enrichment of 1.1 %. In comparison, the CROCUS reactor at EPFL in Switzerland becomes critical at 1.806 % enrichment (Frajtag et al. 2018). For light water, the moderation length is much smaller, and therefore it is much better to distribute the same amount of uranium in many rods of small diameter (as in CROCUS) than in large cubes. This is due to the much larger scattering cross-section of H compared to D. In Table 6, we provide k_{eff} in dependence of different enrichment levels.

6.4 Effect of outer reflector thickness and material

In order to reduce neutron losses, the Haigerloch B8 reactor had a shell of width of 40 cm around the inner vessel made of graphite blocks. In this section, we investigate the influence of the width and of alternative materials of the shell on the effective neutron multiplication factor. The results are shown in Figure 6. As can be seen, k_{eff} grows when the shell thickness is increased. For graphite, the dependence saturates around a thickness of 70 cm, indicating that the optimal width of the reflector was not yet realized, although graphite was available in abundant quantities. Other materials could have been used as reflectors as well, such as beryllium, iron or natural uranium. Their reflection properties are shown in Figure 6 as well. Beryllium would have been slightly superior to graphite because of the (n, 2n) reaction in which beryllium absorbs one neutron and emits two neutrons, which significantly increases the neutron number inside the reactor. Yet, due to the historic circumstances, beryllium was difficult to obtain. The reflection properties of the other two materials iron and uranium are inferior to graphite or beryllium.

Table 6: k_{eff} for natural uranium and enriched UO_2 fuel in the B8 reactor configuration.

Fuel material	k_{eff}
Natural uranium	0.9517 ± 0.00048
UO_2 (0.9 %)	0.9634 ± 0.00045
UO_2 (1.0 %)	1.0062 ± 0.00036
UO_2 (1.1 %)	1.0194 ± 0.00078
UO_2 (1.25 %)	1.0614 ± 0.00044
UO_2 (1.5 %)	1.1227 ± 0.00057
UO_2 (1.6 %)	1.1435 ± 0.00038
UO_2 (2.5 %)	1.2693 ± 0.00061
UO_2 (2.6 %)	1.2780 ± 0.00077
UO_2 (4.5 %)	1.3739 ± 0.00079
UO_2 (4.55 %)	1.3951 ± 0.00059

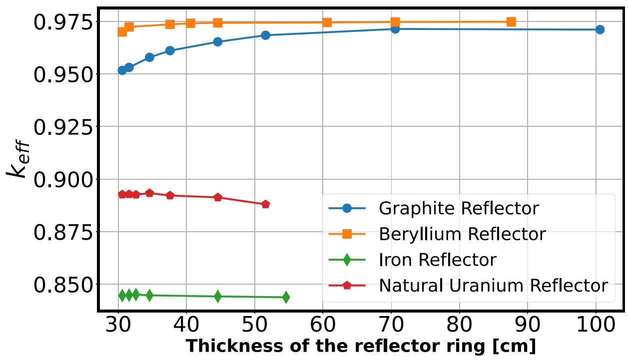

Figure 6: k_{eff} of the Haigerloch B8 reactor as a function of the width of the reflector shell for different reflector materials graphite, beryllium, iron and uranium as indicated. The Haigerloch reactor experiment used graphite.

6.5 Effect of contamination of the heavy water

6.5.1 Light water contamination

In this section, the influence of the contamination of the heavy water as the moderator by light water is examined using historical geometry and materials. The contamination of the heavy water inventory (D_2O) with light water (H_2O) is highly probable, although the precise rate is unknown. The heavy water available in 1945 was produced already in 1941 by Norsk Hydro in Norway. Due to different usage until 1945 and due to potential degradation by absorbing light water present in air as moisture, a contamination by light water is likely. It is therefore important to analyze the influence of light water contamination on the effective neutron multiplication factor of the B8 experiment. In the simulations of the reference case as well as in the parametric calculations presented so far, we have assumed a contamination by 5 % light water. Park (2022) reported that the purity of samples of B8 heavy water kept at NIST was measured at NIST in 1947 to be 96.8 %. So, it is useful to vary the contamination rate and study the influence on criticality. The corresponding results are shown in Table 7 and in Figure 7.

Table 7: Impact of light water contamination on k_{eff} with corresponding errors.

Light water	
Contamination (%)	**k_{eff}**
0 %	0.9749 ± 0.00089
2.5 %	0.9711 ± 0.00079
5 %	0.9517 ± 0.00048
7.5 %	0.9313 ± 0.00078
10 %	0.9092 ± 0.00065
15 %	0.8626 ± 0.00074
20 %	0.8184 ± 0.00066

6.5.2 Boron contamination

A further source of a potentially high-impact contamination of heavy water is boron-10 since it is a strong neutron absorber. Boron enters the aquatic environment through mineral extraction, coal burning, the discharge of wastewater with borax-produced detergents, boron fertilizer/pesticide applications, and the by-burning of boride-treated wood (Liu et al. 2022). In this section, we analyze the impact of boron-10 contamination in the heavy water on the effective neutron multiplication factor in the B8 reactor. The results are shown in Figure 7 and in Table 8. Boron has a strong influence on the effective neutron multiplication factor of the reactor. Even with only 1 ppm contamination of boron-10, the value drops from $k_{\text{eff}} = 0.9517 \pm 0.00048$ with no contamination, to $k_{\text{eff}} = 0.9317 \pm 0.00088$ down to $k_{\text{eff}} = 0.2921 \pm 0.00063$ with 1,000 ppm contamination. The fact that Heisenberg and Wirtz (1947) reported a $k_{\text{eff}} = 0.85$ with $M = 6.7$ may be attributed to a slight contamination of the heavy water used with boron or light water.

7 An optimized Haigerloch reactor design

Heisenberg and Wirtz (1947) estimated in their historic report that an increase of the radius of the inner core vessel from 60 cm to 80 cm would have been sufficient to reach criticality. To improve the reflection properties of the graphite layer, they also suggested to insert uranium “pieces” into the graphite shell. In this section, we shall investigate two optimization strategies, a mere up-scaling of the historic configuration by adding further rings of fuel chains, and a modification of the geometry.

7.1 Scaling of the entire B8 geometry

In order to scale the reactor, we need to assume a realistic enlargement of the reactor. This means that an additional ring with aluminum cables and uranium cubes must be built. This also means that the amount of heavy water and the size of the magnesium vessel, the graphite reflector and the aluminum vessel have to be changed. For simplicity, we keep the height of the reactor as before. To determine the number of the

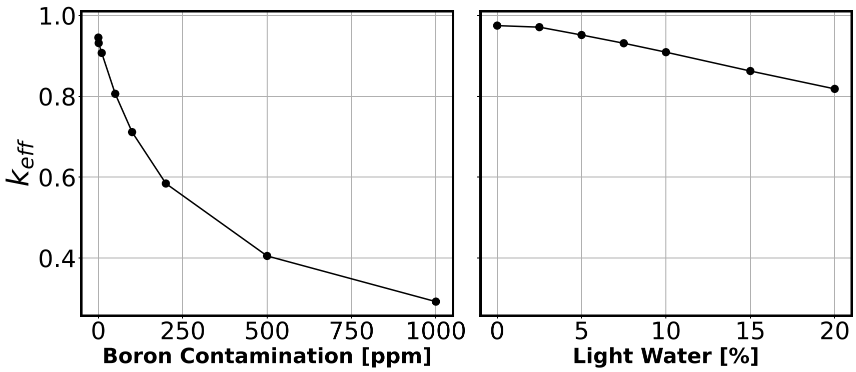

Figure 7: Comparison of the effect of boron (left) and light water (right) contamination in the moderator on the criticality. Even small amounts of boron lead to a more pronounced reduction in k_{eff} than the corresponding levels of light water, illustrating the high neutron absorption efficiency of boron impurities.

Table 8: Impact of the contamination of heavy water with boron on k_{eff}. Each line represents the contamination level in parts per million (ppm). Boron-10 and boron-11 occur in nature in an isotope ratio of 1–4, which is reflected by the mass distribution.

Contamination	Boron-10/-11	k_{eff}
0 ppm	–	0.9517 ± 0.00048
1 ppm	$2.0 \times 10^{-7}/8.0 \times 10^{-7}$	0.9317 ± 0.00088
10 ppm	$2.0 \times 10^{-6}/8.0 \times 10^{-6}$	0.9073 ± 0.00086
50 ppm	$1.0 \times 10^{-5}/4.0 \times 10^{-5}$	0.8062 ± 0.00084
100 ppm	$2.0 \times 10^{-5}/8.0 \times 10^{-5}$	0.7115 ± 0.00081
200 ppm	$4.0 \times 10^{-5}/1.6 \times 10^{-4}$	0.5843 ± 0.00072
500 ppm	$1.0 \times 10^{-4}/4.0 \times 10^{-4}$	0.4051 ± 0.00076
1000 ppm	$2.0 \times 10^{-4}/8.0 \times 10^{-4}$	0.2921 ± 0.00063

suspending wires in the fifth ring of a structure of concentric cylinders, whose total diameter is 115.6 cm and each ring has an effective shell thickness of approximately 14 cm, we first analyze the existing rings. The first ring contains seven cables, the second ring has 15 cables, the third ring has 24 cables, and the fourth ring has 32 cables. These cables are evenly distributed around the circumference of each ring. To see the pattern in the increase in the number of cables, we consider the differences between the rings: from 7 to 15 (with eight more), from 15 to 24 (with nine more), and from 24 to 32 (with eight more). There is an average increase in the number of cables of about 8. Taking this symmetry and the average increase into account, an increase of eight can be assumed for the fifth ring. Therefore, the fifth ring would probably have about 40 cables, which are also arranged symmetrically. This means an increase of 272 uranium cubes with alternating hanging of eight and nine cubes. For each additional ring with an effective thickness of 14 cm, the diameter of the magnesium tank, the graphite reflector and the aluminum tank must increase by 28 cm. The angle of the cable position to an imaginary line through the reactor is adjusted in each case by dividing 360° by the number of cables.

By this we find that an extension by a **fifth ring** with an additional 272 cubes to a total of 936 cubes leads to an increased neutron multiplication factor of k_{eff} = 0.9792 ± 0.00096. This implies a total mass of natural uranium of 2,234.7 kg, which is an increase by 649.4 kg of the original approximately 1,585.3 kg. This corresponds to a multiplication of 1.41 of the uranium mass. In this configuration, the Mg vessel has a radius of 78 cm. The graphite reflector has a radius of 119 cm, the Al tank has a radius of 120 cm, and the overall outer dimension of the reactor is 170 cm. All dimensions are measured radially from the center of the reactor.

As one additional ring is still not sufficient to reach criticality, a **sixth ring** is next added. This increases the number of the uranium cubes by 408 to total 1,344. The effective neutron multiplication factor increases to k_{eff} = 0.9982 ± 0.00083. This implies a total mass of natural uranium of 3,208.8 kg, which is an increase by 1,623.5 kg compared to the original approximately 1,585.3 kg. This corresponds to a scaling factor of 2.02. In this configuration, the Mg vessel has a radius of 93 cm. The graphite reflector has a radius of 134 cm, the Al tank has a radius of 135 cm, and the overall outer dimension of the reactor is 185 cm. The reactor would have come very close to criticality in this set-up with six rings.

For completeness, we investigate how much a **seventh ring** would increase the criticality of the up-scaled B8 reactor further. The seventh ring increases the number of uranium cubes by 476 to total 1,820 cubes. Likewise, this means a total mass of natural uranium of 4,345.25 kg, which is an increase by 2,759.95 kg to the original approximately 1,585.3 kg. This corresponds to a scaling factor of 2.74. In this configuration, the Mg vessel has a radius of 98 cm. The graphite reflector has a radius of 139 cm, the Al tank has a radius of 140 cm, and the overall outer dimension of the reactor is 190 cm. For this configuration the Serpent 2 simulation gives an effective neutron multiplication factor of k_{eff} = 1.0108 ± 0.00090. This reactor would however be prompt supercritical and should never be realized due to safety reasons.

To summarize this part, it would have been required to augment the reactor with at least a sixth ring, corresponding to a scaling factor of **2.02** of the original amount of uranium and a total mass of uranium of 3,208.8 kg, with the same shape and spacing of the uranium cubes. This would have required a radius of the inner core vessel (Mg vessel) of 93 cm. Thus, an increase of the radius of the inner core vessel from 60 cm to 80 cm, as estimated by Heisenberg and Wirtz (1947) (which corresponds to the addition of a fifth ring) would not have been sufficient to reach criticality.

7.2 Variation of fuel element spacing

After exploring scaling scenarios of the historic B8 reactor setup, we now turn to optimization strategies that respect the historical constraint of a limited amount of heavy water. Instead of increasing the reactor size or the number of uranium cubes, this section investigates whether a more favorable spatial configuration of the existing fuel could have improved the effective neutron multiplication factor. Specifically, we analyze the impact of the distance between fuel cubes on k_{eff}, keeping the total heavy water volume constant.

To preserve the overall moderator content while varying the fuel element distance, the radius of the cylindrical core was adjusted accordingly. In order to maintain the geometrical structure of the suspended chains, the height of the core was also varied in proportion to the number of cubes per chain. This ensures that only the spacing between fuel cubes changes, while the overall fuel mass and moderator mass remain fixed. Furthermore, a 5 % contamination of the heavy water with light water was taken into account in all calculations to realistically reflect the historical boundary conditions.

The results, presented in Table 9 and Figure 8, show that k_{eff} reaches a maximum at a fuel element distance of approximately 14 cm. Although a larger spacing increases the moderator volume between the cubes and improves moderation, it also raises the probability of neutron absorption in the light water component. This trade-off leads to an optimum configuration at 14 cm, where the fuel-to-moderator ratio and reflector conditions are most favorable. These findings indicate that the original B8 design was already close to the optimal spacing with respect to the achievable effective neutron multiplication factor under the material constraints of the time.

Our investigations also show that, assuming completely pure heavy water, the original B8 configuration with a fuel element spacing of 14 cm and the corresponding cylindrical core dimensions would lead to a significantly higher value of $k_{eff} = 0.98209 \pm 0.00078$. This underlines the strong influence of the moderator purity on the neutron economy, which is mainly due to the significantly higher absorption cross section of hydrogen compared to deuterium.

Table 9: k_{eff} as a function of the distance between fuel cubes, together with the corresponding fuel chain lengths and core dimensions in the Haigerloch reactor model. The core radius and height are adjusted to maintain a constant amount of heavy water, while preserving the geometric structure of the suspended cube chains. A light water contamination of 5 % is included to reflect historical conditions.

Fuel element distance	Fuel chain length	Core radius	Core height	k_{eff}
9.0 cm	81.0 cm	73.8 cm	81.0 cm	0.92052 ± 0.00081
10.0 cm	90.0 cm	70.0 cm	90.0 cm	0.93107 ± 0.00031
11.0 cm	99.0 cm	66.8 cm	99.0 cm	0.94133 ± 0.00052
12.0 cm	108.0 cm	63.9 cm	108.0 cm	0.94609 ± 0.00048
12.5 cm	112.5 cm	62.6 cm	112.5 cm	0.94722 ± 0.00089
13.0 cm	117.0 cm	61.4 cm	117.0 cm	0.94797 ± 0.00084
13.5 cm	121.5 cm	60.3 cm	121.5 cm	0.95058 ± 0.00099
14.0 cm	126.0 cm	59.2 cm	126.0 cm	0.95284 ± 0.00037
14.5 cm	130.5 cm	58.2 cm	130.5 cm	0.95059 ± 0.00064
15.0 cm	135.0 cm	57.2 cm	135.0 cm	0.94863 ± 0.00059
15.5 cm	139.5 cm	56.2 cm	139.5 cm	0.94715 ± 0.00047
16.0 cm	144.0 cm	55.4 cm	144.0 cm	0.94545 ± 0.00070
17.0 cm	153.0 cm	53.7 cm	153.0 cm	0.93642 ± 0.00032
17.5 cm	157.5 cm	52.9 cm	157.5 cm	0.92331 ± 0.00046
18.0 cm	162.0 cm	52.2 cm	162.0 cm	0.92279 ± 0.00082

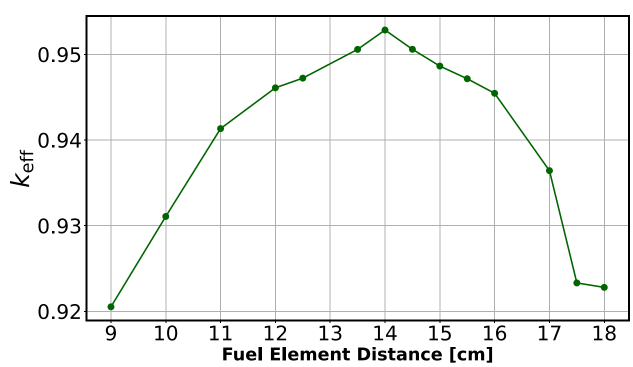

Figure 8: Variation of k_{eff} as a function of the fuel element distance. The amount of heavy water was kept constant by adjusting the reactor core radius and the core height according to the chain length, which depends on the fuel element spacing. A maximum k_{eff} was observed at a distance of approximately 14 cm.

These results suggest that the historical B8 configuration was already very close to criticality under more favourable conditions. This raises the question of whether criticality could have been achieved by adjusting the reactor geometry, especially assuming that pure heavy water is available. In the following, we therefore investigate modified core geometries that retain the basic design principles but offer improved neutron moderation and reflection. This could also allow a reduction in the amount of fuel while still achieving the critical threshold.

7.3 Adjusting the geometry

Pešić (2018) showed that a modification of the geometry of the reactor core, which contains both uranium and heavy water, by increasing the diameter from 115.6 cm to 160 cm and simultaneously reducing the height from 169 cm to 160 cm can lead to an increase in the effective neutron multiplication factor. All other parameters, such as the materials used and the wall thickness of the Mg and Al vessels, remained unchanged. The wall thickness of the graphite reflector was set to 40 cm and was also not changed, taking into account the stacking of the graphite blocks in the reflector. This change in geometry increases the total moderator volume, thus allowing a larger amount of heavy water to be used. In line with the assumptions of Pešić (2018), it was further assumed that the heavy water was completely pure.

7.3.1 664 uranium cubes

First, we use 664 cubes with the new dimensions in the original staggered arrangement to examine the dependence of the effective neutron multiplication factor on the distances between the cubes. Parametric calculations were performed with Serpent 2 varying the distances between cubes. In each calculation the same value was used for the horizontal (referring to the position of the Al cables) and the vertical direction. The results are shown in Figure 9.

It can be seen that k_{eff} generally increases with increasing edge length, which is due to the fact that more uranium is present in the reactor core with a larger edge length. A larger fuel mass means more fissile material, which increases the probability of neutron interactions and thus increases k_{eff}. However, this increase is not linear, and an interesting behavior can be observed at a distance of 15 cm.

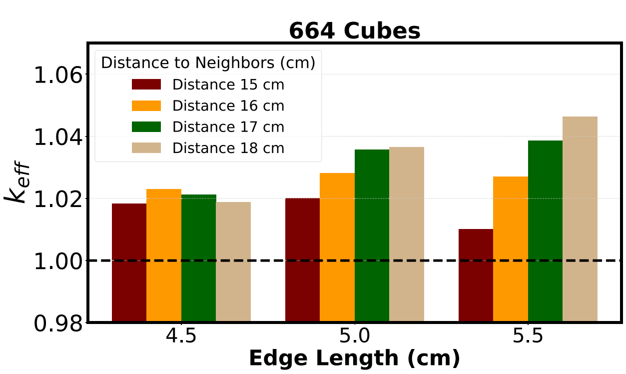

Figure 9: Effect of edge length and distance to the next neighbors on k_{eff} with 664 uranium cubes. The results show that both the cube edge length and spacing strongly influence the fuel-to-moderator ratio and the effective neutron multiplication factor For this configuration, all tested combinations result in $k_{\mathrm{eff}} > 1$, indicating supercriticality.

In this case, k_{eff} reaches its maximum at an edge length of 5.0 cm with $k_{\mathrm{eff}} = 1.0201 \pm 0.00075$. For edge lengths of 4.5 cm ($k_{\mathrm{eff}} = 1.0183 \pm 0.00056$) and 5.5 cm ($k_{\mathrm{eff}} = 1.0101 \pm 0.00081$), the effective neutron multiplication factor is lower. This shows that at an edge length of 5.0 cm, the ratio of fuel quantity and moderator volume is optimal. A smaller edge length means that there is more moderator, but the amount of fuel is too small to achieve maximum criticality. A larger edge length, as with 5.5 cm, offers more fuel, but the space for the moderator between the cubes becomes too small to efficiently slow down neutrons, which leads to a drop in k_{eff}.

A similar pattern can be seen at a distance of 18 cm. Here, k_{eff} is maximal at an edge length of 5.5 cm (k_{eff} = 1.0463 ± 0.00077). The larger distance allows the moderator to have enough space to optimally decelerate the neutrons, resulting in a larger effective neutron multiplication factor. For smaller edge lengths, such as 5.0 cm ($k_{\mathrm{eff}} = 1.0366 \pm 0.00082$) and 4.5 cm ($k_{\mathrm{eff}} = 1.0189 \pm 0.00062$), the effective neutron multiplication factor decreases slightly because the moderator-fuel mix is less efficient, although the larger distance allows good moderation in principle.

With an edge length of 4.5 cm, k_{eff} reaches its maximum value of $k_{\mathrm{eff}} = 1.0230 \pm 0.00071$ at a distance of 16 cm to the nearest neighbor. For an edge length of 5 cm, the maximum value of k_{eff} is $k_{\mathrm{eff}} = 1.0366 \pm 0.00082$ at a distance of 18 cm. With an edge length of 5.5 cm, k_{eff} reaches its maximum value of $k_{\mathrm{eff}} = 1.0463 \pm 0.00077$ at a distance of 18 cm.

It is clear that there is an optimum in the ratio of fuel quantity and moderator availability. This optimum is determined both by the edge length of the fuel cubes and by the distance between them. Yet, obviously, k_{eff} is well above 1, indicating that the reactor would be supercritical. Hence, obviously the number of fuel cubes can still be decreased, as investigated in the subsequent sections.

7.3.2 508 uranium cubes

When the number of uranium cubes is reduced to 508, we investigate the cases of the edge length of 4.5 cm and 5 cm arranged at different distances. This corresponds to a mass of 882 kg for an edge length of 4.5 cm and 1,210 kg for an edge length of 5 cm. The results of the effective neutron multiplication factor is shown in Figure 10. With an edge length of 4.5 cm and a distance of 18 cm, we already have a result here that, with $k_{\mathrm{eff}} = 0.9998 \pm 0.000043$, is very close to 1 and has a uranium mass of only 882 kg.

7.3.3 430 uranium cubes

Since cubes with an edge length of 5 cm were available and $k_{\mathrm{eff}} > 1$ for the case of 508 cubes, it is possible to reduce the

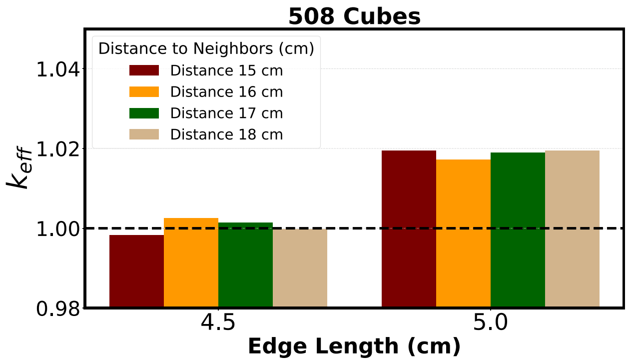

Figure 10: Effect of edge length and distance to the next neighbors on k_{eff} with 508 uranium cubes. The optimal configuration with an edge length of 4.5 cm and a spacing of 18 cm results in $k_{\text{eff}} = 0.9998 \pm 0.000043$, despite the significantly reduced fuel mass of 882 kg.

number of cubes even further. We show that a further reduction 430 cubes is possible, which corresponds to a mass of 746 kg for an edge length of 4.5 cm and a mass of 1,024 kg for an edge length of 5 cm. The results for k_{eff} are shown in Figure 11.

For an edge length of 4.5 cm, there is too little uranium in the reactor, while for an edge length of 5 cm, an optimum is found near $k_{\text{eff}} = 1$ at 16 cm distance with $k_{\text{eff}} = 0.9998 \pm 0.00062$.

To summarize, with the results for an edge length of 4.5 cm, 508 cubes with a total mass of 882 kg and a heavy water volume of 3,170 L, and $k_{\text{eff}} = 0.9998 \pm 0.000043$, and for the configuration with an edge length of 5 cm, 430 cubes with a total mass of 1,024 kg and a heavy water volume of 3,162 L, and $k_{\text{eff}} = 0.9998 \pm 0.00062$, show that both configurations are very close to the optimal $k_{\text{eff}} = 1$. Under the condition to use as little uranium and heavy water as possible, the configuration with an edge length of 4.5 cm and a distance of 18 cm would be the optimal choice, while under the condition to use the already existing cubes with an edge length of 5 cm, they would have to be arranged at a distance of 16 cm. The amount of about 3,170 L of heavy water has to be compared to the available amount of 1,360 L (Bopp et al. 1945). An amount of almost two-and-a-half times the available quantity would have been necessary to reach criticality. In both cases, we can conclude that the bottleneck of the B8 experiment was not the lack of uranium, but the lack of heavy water.

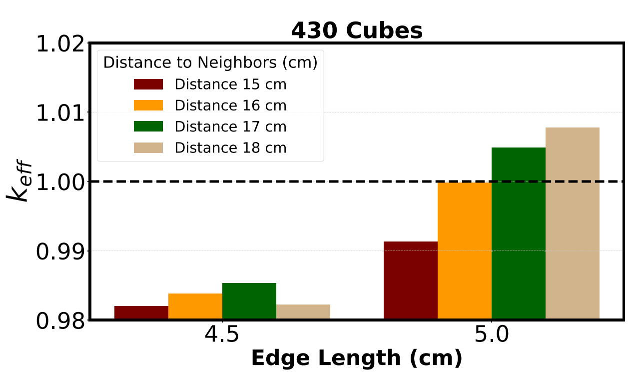

Figure 11: Effect of the edge length and the distance to the next neighbors on k_{eff} with 430 uranium cubes. For a cube size of 5 cm, criticality is nearly reached at a spacing of 16 cm with $k_{\text{eff}} = 0.9998 \pm 0.00062$, while smaller cubes fall short due to insufficient fuel mass.

Furthermore, it must be emphasized that operating the reactor in this configuration would neither have been advisable nor permissible under today's safety standards. Due to the reduced amount of fuel and the slightly increased amount of moderator, an unfavorable moderator-to-fuel ratio

$$\frac{N_{\text{Mod}}}{N_{\text{Fuel}}}$$

results, leading to overmoderation. This may cause the reactivity to increase with rising temperature, as the density of the moderator decreases. Such behavior poses a significant safety risk, as it can lead to a positive feedback effect and, consequently, to potential reactor instability.

7.4 Optimzed B8 configuration

Consequently, we may conjecture two optimized B8 reactor configurations (set-up A and B) which should have had the following configurations:

- Height of the reactor core/Mg vessel: 160 cm
- Diameter of the reactor core/Mg vessel: 160 cm
- Type of fuel: Natural uranium cubes
- Edge length of uranium cubes: 4.5 cm (A) or 5 cm (B)
- Number of uranium cubes: 508 (A) or 430 (B)
- Mass of uranium cubes: 882 kg (A) or 1,024 kg (B)
- Number of rings for cable suspension: 4
- Arrangement of the rings: Concentric
- Number of cables: 78
- Number of uranium cubes per cable: 7 and 6
- Arrangement of uranium cubes: Staggered
- Distance between uranium cubes or cables in x, y, z direction: 18 cm (A) or 16 cm (B)
- Type of reflector: Graphite
- Wall thickness of the graphite reflector: 40 cm
- Impurities in the reflector: None
- Stacking of graphite reflector blocks: With gaps, as in the historical reactor
- Amount of heavy water: 3,170 L (A) or 3,162 L (B)
- Impurities of heavy water with light water: None

8 Summary and conclusion

We have simulated the effective neutron multiplication factor of the historic Haigerloch B8 nuclear reactor using contemporary Serpent 2 Monte Carlo simulations. The input parameters of the reactor configurations were taken from historic reports, from direct measurements of the replica of the reactor at the Haigerloch Atomkeller museum or taken from literature. We find an effective neutron multiplication factor of $k_{\text{eff}} = 0.952$ which coincides with previously calculated results reported by two other groups in the literature. Remarkably, all calculated values are larger than the historically reported measured value of $k_{\text{eff}} = 0.85$ reported by Heisenberg and Wirtz (1947). We point out that no original reports from April 1945 exist anymore. The reason for the discrepancy remains unclear at present.

We have systematically tuned device parameters, such as the side length of the uranium cubes and their distance. It turns out that the size of the uranium cubes used (also given the historic circumstances) was close to the optimum. We also find that the use of uranium with 1 % enrichment would have turned the reactor critical. Furthermore, we tuned the width and the material of the reflector shell. We find that graphite shows the best properties given the historic situation. An increase of the width from 40 cm to 70 cm would have only slightly increased the effective neutron multiplication factor, albeit the reactor would still remain below criticality.

We also studied the dependence on contamination of the heavy water with light water and boron. Yet, historic measurements of the purity of heavy water reported by Park (2022) show a D_2O purity of 96.8 %.

In addition, we have analyzed whether an alternative spatial arrangement of the fuel cubes could improve the effective neutron multiplication factor, while keeping the amount of heavy water constant. To do so, the spacing between the uranium cubes was systematically varied, while the reactor core radius and height were adjusted accordingly to preserve the total volume of the moderator. A light water contamination of 5 % was assumed to reflect historical conditions. We find that an optimal fuel element distance of about 14 cm maximizes k_{eff}. If instead pure heavy water had been available, the original geometry would have yielded a significantly higher value of $k_{\text{eff}} = 0.98209 \pm 0.00078$, indicating that the historical configuration was already close to criticality. This motivates further investigation into geometric optimization strategies that maintain the reactor type but improve the neutron economy.

Finally, we studied a possible optimization of the historic B8 reactor. The procedure carried out here is not unique and guided by the historic fact that the material of the fuel and the moderator was sparse and that the overall type of the reactor remains unchanged. We find an optimized reactor with a slightly increased diameter of the core from 120 cm to 160 cm while keeping its height. The amount of uranium fuel can even be decreased, but the crucial factor is that the amount of heavy water is increased from 1,360 L to 3,170 L, i.e. by a factor of 2.33. This clearly shows that the limiting factor was the lack of heavy water, while the available fuel was more than enough and the general approach of the reactor design would have been successful.

The reactor design has several parameters which can be tuned, but not all of them are equally relevant. It is reasonable to assume that Heisenberg and Wirtz had realized the dominant importance of heavy water as a moderator. Before they designed the configuration of the Haigerloch B8 reactor, the decisive historic circumstance was the availability of the limited amount of heavy water. Later reports mention that about 1.5 to of heavy water were transported to the U.S.A., which corresponds to about 1360 L (in this estimate, we ignore the fact that the heavy water had a purity of 96.8 %, as was measured in samples of B8 heavy water kept and measured at NIST in 1947 (Park 2022); furthermore we assume a density of $\rho_{D_2O} = 1.1047$ kg/L). It seems plausible that the B8 reactor was constructed such that this available amount of heavy water could be used to fill the inner vessel entirely. The volume of the inner cylinder with a diameter of 116 cm and a height of 132 cm amounts to 1,395 L, from which the volume of the 664 uranium cubes of side length of 5 cm, which is 83 L, has to be subtracted. So the overall volume of possible heavy water amounts to 1,312 L, which agrees well with the available amount of 1,360 L.

An interesting perspective is a more detailed comparison of the Haigerloch B8 device with the Chicago Pile CP-1, which has reached criticality already in 1942. In a recent study, Zoia et al. (2025) have used the Monte Carlo particle transport code TRIPOLI of CEA to determine the effective neutron multiplication factor. Actually, a good agreement between historically reported experimental results and modern simulation results has been reached (Zoia et al. 2025). A direct quantitative comparison of the CP-1 and the Haigerloch B8 devices is not straightforward, because both obviously follow from very different design strategies. The CP-1 consists of layers of uranium plates and graphite as moderator. No heavy water was used. The strategy behind the Haigerloch B8 design was most likely focused on better moderator properties using heavy water and better reflection properties. It seems that rather careful optimization was carried out under the premise that only a limited amount of heavy water was available and the precise amount of fuel was secondary. In contrast, the design strategy of CP-1 followed the route to use a large amount of easily available uranium fuel and graphite, avoiding heavy water. Not much care was given to optimization and the dimensions of the device were just made large.

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