Optimization of a compact D-D fast neutron generator for imaging applications

A thesis submitted to attain the degree of
DOCTOR OF SCIENCES of ETH ZURICH
(Dr. Sc. ETH Zurich)

presented by

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2020
Meinen Eltern: Helena und Rudolf.
Acknowledgments

Above all, I would like to express my deep gratitude to Prof. Dr. Horst-Michael Prasser for his scientific leadership throughout this project as well as for the many discussions and creative ideas that improved the scientific quality of this work. I also wish to thank Dr. Robert Adams for his strenuous, dedicated day-to-day contributions and encouraging support that helped overcome the many hurdles throughout this journey. My gratitude also extends to Dr. Robert Zboray for his guidance and support. Furthermore, I thank Prof. Dr. Karl van Bibber, Dr. Chris Franklyn, and Dr. Cédric Carasco for co-examining this work and their critical review.

My gratitude also extends to Benoît Soubelet, who turned from PSI officemate to dear friend. I was extremely lucky to have had outstanding secretaries at PSI, Andrea Mohr, and at ETH, Fiorella Meyer. I am very grateful to them for they enabled me to minimize my time spent in administrative processes. Many of the milestones achieved in this work were directly or indirectly related to the generous practical support from Max Fehlmann, Wilhelm Bissels, and Simon Suter. Support from Dr. Domenico Paladino, Dr. Gregory Perret, and Alexander Wolfertz of the experimental thermal-hydraulics group at PSI was also essential and is greatly appreciated. I would furthermore like to thank Dietmar Götz, Tobias Albrecht, and Tobias Makiola at PSI for providing the design of the microwave ion source and for their help to adopt it successfully.

I would also like to thank my colleagues at ETH Abhishek Saxena, Lukas Robers, Nathan Lafferty, Petros Papadopoulos, and Xiaorong Li for their humour and collegiality. I also wish to thank the Swiss National Science Foundation (SNSF, grant number 200021-162411/1) for the generous financial support.

I am tremendously grateful for the unconditional support, timely encouragement, and endless patience of my parents. I am also most grateful for the care and backing of family and friends. Finally, I am peculiarly thankful to Seraina for the many hours in our weekendoffice and for always being there for me.

Heiko Kromer
Zürich | April 20, 2020
Abstract

In this thesis efforts of optimizing a compact deuterium-deuterium (D-D) fast neutron generator with an emphasis on neutron transmission-based imaging applications are outlined. The main objective was the development and thorough characterization of a high output neutron source with a small neutron emitting spot size.

The study is divided into three main sections. In the first part a novel, water-cooled, drive-in rotating beam target was developed, designed, and implemented. The optimized beam target configuration was found using extensive computational fluid dynamics and heat transfer analyses. During experiments, no indication of loss of deuterium due to outgassing was observed with the 40 mm diameter, rotating copper rod that was coated with 5 \( \mu \)m of titanium. At a rotational velocity of 220 rpm the stable neutron output was increased to \( 2.9 \times 10^7 \text{s}^{-1} \), which was an increase by a factor of more than four compared to the neutron output with a stationary titanium target.

In the second main section of this thesis the thorough characterization of the compact D-D neutron generator is presented in terms of overall neutron output and neutron emitting spot size. Both of these variables are extremely important characteristics of a neutron generator tailored to transmission-based imaging methods. Estimation of the overall neutron output was achieved by combining a detailed Monte Carlo model of the neutron source and its surroundings with the reading of an LB6411 neutron probe. The neutron emitting spot size was indirectly measured using an attenuating edge technique where a tungsten block was moved in between the path of direct neutron emission and a detector. The results of the attenuating edge measurements were benchmarked using charged particle tracing simulations with COMSOL Multiphysics. These simulations estimated the distribution of deuterium ions on the surface of the target rod.

The third main section describes the design, implementation, and performance of a major design iteration of the compact D-D fast neutron generator. Charged particle tracing simulations were set up to optimize the geometry and dimensions of the neutron generator with respect to ion spot size on the target surface. The goal of further increased neutron output was realized by raising the accelerating potential limit that was achieved
by improving the vacuum quality. This included the design of an optimized generator housing and adoption of an electron cyclotron resonance microwave ion source which enabled operation of a deuterium plasma at lower gas pressure levels than the previous radio frequency-based ion source design. The use of an electric field driven electron suppression using an added suppression electrode succeeded in reducing backstreaming secondary electrons from the target, which helped in reduction of high voltage breakdown probability and greatly increased stability of operation of the neutron generator. With all these efforts, the stable neutron output at $-120$ kV was increased in total by a factor of eight to $6 \times 10^7$ s$^{-1}$ in comparison to what was achieved before the start of this thesis work. At the highest accelerating potential of $-145$ kV that was achieved without significant high voltage breakdowns the peak neutron yield was $6.8 \times 10^7$ s$^{-1}$. Using the attenuating edge measurement technique, the emitting spot size was determined to be in the range of 2 to 3 mm. This represents a dramatic improvement in imaging performance potential of the neutron generator compared to the starting point of this work.
Zusammenfassung


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<th>Meaning</th>
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<tr>
<td>2D</td>
<td>Two-Dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>Three-Dimensional</td>
</tr>
<tr>
<td>CAD</td>
<td>Computer Aided Design</td>
</tr>
<tr>
<td>CCD</td>
<td>Charge-Coupled Device</td>
</tr>
<tr>
<td>CDF</td>
<td>Cumulative Distribution Function</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
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<tr>
<td>CuCrZr</td>
<td>Copper-chromium-zirconium</td>
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<tr>
<td>CuOFE</td>
<td>Oxygen-free high conductivity copper</td>
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<tr>
<td>D-D</td>
<td>Deuterium-Deuterium</td>
</tr>
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<td>D-T</td>
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<tr>
<td>ESF</td>
<td>Edge Spread Function</td>
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<tr>
<td>ETH</td>
<td>Eidgenössische Technische Hochschule (Swiss Federal Institute of Technology) Zürich</td>
</tr>
<tr>
<td>FKM</td>
<td>Fluorelastomer</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full Width at Half Maximum</td>
</tr>
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<td>IAEA</td>
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<tr>
<td>ISNR</td>
<td>International Society for Neutron Radiography</td>
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<tr>
<td>MCNP6</td>
<td>Monte Carlo N-Particle code version 6</td>
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<td>NPi</td>
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<td>PSI</td>
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<tr>
<td>PVT</td>
<td>Polyvinyl Toluene</td>
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<tr>
<td>RF</td>
<td>Radio-Frequency</td>
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<tr>
<td>RFQ</td>
<td>Radio-Frequency Quadrupole</td>
</tr>
<tr>
<td>SiPM</td>
<td>Silicon Photo Multiplier</td>
</tr>
<tr>
<td>SRIM</td>
<td>Stopping Power and Range of Ions in Matter</td>
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## Physical Constants

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<td>( b = 10^{-28} \text{ m}^2 ) [1]</td>
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<td>Electron charge</td>
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<td>Unified atomic mass</td>
<td>( u = 1.660 , 539 , 040 \times 10^{-27} \text{ kg} ) [1]</td>
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<td>Deuteron mass</td>
<td>( m_D = 2.013 , 553 , 212 , 745 \text{ u} ) [2]</td>
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<td>( N_A = 6.022 , 140 , 857 \times 10^{23} \text{ mol}^{-1} ) [1]</td>
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## Symbols

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<tr>
<td>$AlN$</td>
<td>Alumina</td>
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</tr>
<tr>
<td>$B_o$</td>
<td>Overall resolution</td>
<td>mm</td>
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<td>Image blur induced by finite emitting spot</td>
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</tr>
<tr>
<td>$B_{do}$</td>
<td>Image blur induced by detector</td>
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<td>$Be$</td>
<td>Beryllium</td>
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<td>$C$</td>
<td>Count rate</td>
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<td>$I_{ion}$</td>
<td>Averaged current due to deuterium ion beam</td>
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<td>$I_{leak}$</td>
<td>Averaged leakage current</td>
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<td>$j$</td>
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<td>Number of source particles set in MCNP6</td>
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</tr>
<tr>
<td>$P$</td>
<td>Power</td>
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<tr>
<td>$R_{tot}$</td>
<td>Total reaction rate per MCNP6 source particle</td>
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</tr>
<tr>
<td>$R_x$</td>
<td>Sputtering yield of compound $x$</td>
<td>atoms ion$^{-1}$</td>
</tr>
<tr>
<td>$R(\theta)/R(90^\circ)$</td>
<td>Neutron yield relative to 90$^\circ$ emission angle</td>
<td>-</td>
</tr>
<tr>
<td>$R(\epsilon)$</td>
<td>Neutron fluence response for neutron energy $\epsilon$</td>
<td>counts per fluence</td>
</tr>
<tr>
<td>$S_c$</td>
<td>Sputter rate of compound $c$</td>
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</tr>
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<td>$Q$</td>
<td>Reaction Q-value</td>
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<tr>
<td>$t$</td>
<td>Time</td>
<td>s</td>
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<td>$T$</td>
<td>Temperature</td>
<td>$^\circ$C</td>
</tr>
<tr>
<td>$T(\epsilon)$</td>
<td>Averaged neutron flux per energy bin $\epsilon$</td>
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<tr>
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<td>Titanium</td>
<td>-</td>
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<tr>
<td>$U$</td>
<td>Uranium</td>
<td>-</td>
</tr>
<tr>
<td>$U_{el}$</td>
<td>Electric potential</td>
<td>V</td>
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<tr>
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<td>Volume</td>
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<td>$Y$</td>
<td>Total neutron yield</td>
<td>s$^{-1}$</td>
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<tr>
<td>Symbol</td>
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<tr>
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<td>--------------------------------------------------</td>
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<td>Spatial position</td>
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<td>$^4\text{He}$ particle</td>
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<td>Attenuation coefficient</td>
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<td>Density</td>
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<td>$\sigma$</td>
<td>Microscopic cross section</td>
<td>barn</td>
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<td>Macroscopic cross section</td>
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<td>$\Phi$</td>
<td>Flux</td>
<td>cm$^{-2}$ s$^{-1}$</td>
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Chapter 1

Introduction

Neutron imaging has become an increasingly popular non-destructive examination tool, with many applications in industry and research [3]. However, neutron imaging is lagging behind X-ray and gamma radiation-based methods for industrial uses due to problems such as limited source strength, poor detector performance, high cost or complexity, and limited source portability. A difficulty connected with a limited flux is the inability to do high-speed pulsed neutron imaging. Large sized neutron sources, discussed in Section 1.1.1, are immobile and offer no practical solution for many situations.

This work focuses in particular on transmission-based imaging where a radiation beam — e.g. X-ray, gamma, or neutron — is attenuated as it passes through a sample (imaging object) [4]. In such an imaging configuration, ideally a detector measures what fraction of radiation emitted by a source passes through the sample without interacting. For each source-detector ray, the attenuation will depend on the contents of the sample along that line. The spatial distribution of that attenuation constitutes a radiographic image, which gives information about the inner structure of the sample. The intensity measured by the detector ideally follows the Beer-Lambert law of attenuation. This law describes the probability of interaction of a particle beam with matter in the sample and reads [5]:

\[
I = \int_{E_0}^{E_1} I_0 (E) \exp \left[ \int_0^d \mu (E, x) \, dx \right] \, dE, \tag{1.1}
\]

where \(I\) denotes the intensity of the beam after passing through the sample, \(I_0\) is the intensity before the sample, \(E\) is the energy of the beam, \(d\) the thickness of sample the beam has to pass along its trajectory, \(\mu\) is the attenuation coefficient, and \(x\) denotes the
spatial position in the sample. Additionally, scattered radiation is usually superposed to the useful signal, which may cause a certain deterioration of the imaging quality.

![Figure 1.1: Illustration of beam transmission-based imaging](image)

The beam intensity before and after the imaging object (sample) can be computed from Equation 1.1.

Non-destructive examination techniques using X-rays and gamma sources are mature and well established in the industry. Wang [6] gives a concise general overview of industrial tomography applications, e.g. the flow-rate measurement of oil-gas-water multiphase flows in the oil and gas industry, or microstructure investigations in the food industry. Nevertheless, for some industrial and research applications X-ray and gamma radiation-based methods are of limited use. In the case of imaging a light element (low atomic number, \(Z\)) that is contained inside an object made of a heavy element (high-\(Z\) number), X-ray and gamma radiation-based methods can produce insufficient contrast, because the attenuation of photons is highly dependent on the \(Z\) number and density of the material. Lower energy photons over-proportionately get removed when the high-\(Z\) part of the material hardens or starves the beam. These lower energy photons would have been needed to see significant image contrast from light elements. In the case of neutron imaging, cold and thermal neutrons show a high sensitivity to specific elements, some of them light, and can still penetrate rather large thicknesses of many heavy elements [7]. Yet, because of this high sensitivity, imaging of objects with a high content of these particular high-attenuation light elements becomes difficult with thermal or cold neutrons. Perfect et al. [8] have shown that while thermal neutrons are suitable for imaging hydrogen-rich fluids (e.g. water and oil) within porous media, their high sensitivity to hydrogen makes them unusable for water thicknesses beyond around 1 cm. Fast neutrons (in the MeV energy range) exhibit usually a much higher penetration power compared to cold and thermal neutrons (and X-rays or gamma radiation). This makes
the imaging of robust and voluminous objects that contain low-Z materials (e.g. water) shielded by a large quantity of high-Z materials (e.g. some cm of steel) possible.

1.1 Types of Neutron Sources for Neutron Imaging

1.1.1 Large and Medium Scale Sources

Large scale neutron sources include research reactors and spallation sources [9]. Spallation neutron sources are typically pulsed neutron sources where a proton beam is accelerated to high energies (in the order of MeV to GeV) and hits a heavy target (e.g. tungsten or lead). For a lead target and a proton beam at 600 MeV around ten neutrons are liberated per incident proton [10]. In a reactor-based neutron source, the neutrons are produced by a self-sustaining series of fission reactions, where neutrons from fission events are diverted to a continuous or pulsed neutron beam. Most of the beamlines at large scale facilities use cold or thermal neutrons (e.g. ANTARES at FRM-2 reactor in Germany [11], ICON and NEUTRA at SINQ spallation source in Switzerland [12]), hence these large systems typically include one or more moderators, filters, apertures, beam limiters, sample manipulator, and a detector system [13]. However, the individual layout of the facility varies greatly and depends strongly on the specific use case. A 2016 report prepared jointly by ISNR and IAEA lists around 48 large scale neutron imaging facilities worldwide [14]. At the end of 2019, at least two neutron imaging facilities have been shutdown (BER-2 reactor in Germany [15] and Orphée reactor in France [16]), but also at least two new research reactors (AR-10 in Argentina [17] and JRTR in Jordan [18]) that plan to include neutron imaging facilities have been constructed since the report was last updated. However, in the overall trend, due to the old age of the reactors, the number of large neutron sources worldwide is dwindling and so is the total accessible beam time from them [12]. Consequently, the many stakeholders from industry and science that are sharing access to beam time compete with one another in proposal procedures. This trend increases the attractiveness and potential of custom-made, application-tailored neutron sources that can produce acceptable neutron flux intensities. On top of a more competitive environment, large scale sources are unsuited for applications requiring a low cost, compact, and/or monoenergetic neutron source. Especially due to their size, large scale sources can by definition not be used for certain in-field applications — e.g. oil well logging [19], homeland security [20, 21], or quality control in industrial processes [22] — that require portable sources.
In the context of large scale sources producing fast neutrons, the neutron flux intensity at a measurement position is typically around $10^7 \text{cm}^{-2}\text{s}^{-1}$ \[13\]. At the beam-lines focusing on imaging with fast neutrons, most studies were performed by using a Charge-Coupled Device (CCD) to collect the neutron induced scintillator light (e.g. Mikerov and Waschkowski \[23\], Takenaka et al. \[24\], or Bücherl et al. \[25\]). The scintillator material is typically hydrogen-rich and scintillation light from the recoil proton is collected and used for image production. These imaging systems typically achieve a resolution of around 1 to 2 mm, limited by the thickness of the scintillator screen which must be reasonably thin to keep blur acceptable, at the cost of a comparably low efficiency. Types of scintillators include, among others, plastic fiber screens \[26\], wavelength-shifting fiber converters \[27\], and polypropylene mixed with zinc sulphide phosphor \[28\]. Typically at research reactors that produce neutrons via the fission reaction, the high gamma radiation presence in the beam causes challenges for the detector design, as the fission reaction of $^{235}\text{U}$ releases approximately 2.44 neutrons and 6.6 gamma photons \[28\]. This requires the use of filters to preferentially suppress gamma radiation, e.g. with lead. Nevertheless, a wide array of research with cold, thermal, and fast neutrons is conducted at large scale sources using radiography, computed tomography, energy selective imaging, and other techniques that are under development \[13\]. Additionally, industrial type of research is conducted, e.g. testing soot particle filters for diesel engines \[29\], visualization of oil lubrication in clutches \[30\], or fuel cell research \[31\]. Further applications include the study of cultural heritage objects \[32\], soil physics \[33\], and investigation of thermal hydraulic phenomena \[34\].

While being smaller compared to large scale sources, the class of sources defined in this work as medium sized (although some are referred to as “small”, for example by the International Collaboration on Advanced Neutron Sources) mostly use particle accelerators to bombard one light element with another to liberate neutrons. These particle accelerators operate typically in the MeV acceleration range to overcome the high threshold energy (arising from a negative reaction $Q$-value) required to initiate some reactions or to achieve high neutron outputs for non-threshold reactions (considered as any reaction positive $Q$-value, such that any threshold is typically negligible). For many industrial applications, the $^1\text{H} + ^7\text{Li} \rightarrow ^7\text{Be} + n$ reaction with a $Q$-value of $-1.64\text{MeV}$ has been considered, since neutrons with less than 0.1 MeV can be produced with a forward peaked bias allowing higher utilization of the neutrons and making radiation shielding more efficient. Chichester \[35\] and Drosg \[36\] give an overview over a variety of possible neutron producing reactions in accelerator driven sources and potential applications of these systems. Exothermic nuclear reactions, such as the deuterium-deuterium (D-D) nuclear reaction, are also used in medium sized sources. Hall et al. \[37\] developed a high-energy neutron imaging system with neutron energies of around 10 MeV. This
accelerator driven D-D neutron source was planned to use a compact radio-frequency
quadrupole (RFQ) to accelerate deuterons at up to 7 MeV and with an average ion
current of 325 µA towards a high pressured (around 3 bar) deuterium gas target. More
compact, but still with a large footprint of around $4 \times 2 \times 1 \text{ m}^3$ and a weight of almost
2000 kg was the commercial high flux D-D neutron source used for radiography in Tay-
lor et al. [38]. The system used a 300 kV high voltage power supply and bombarded a
1 m long, around 20 cm (8 inches) diameter deuterium gas target (kept at a pressure of
approximately 20 mbar) with a deuterium ion beam current of up to 35 mA. The total
neutron output of this system was $5 \times 10^{11} \text{s}^{-1}$. Hamm [39] developed a very compact
RFQ-based commercial neutron source. The smallest model with a length of 1.35 m and
a weight of 350 kg was based on the $^2\text{H} + ^9\text{Be} \rightarrow ^{10}\text{Be} + n$ reaction ($Q$-value 4.361 MeV)
where a 0.9 MeV deuterium ion beam with a maximum ion beam current of 140 µA was
hitting a thick beryllium target. The produced neutrons had a maximum energy of
5.5 MeV at a total neutron output of $1 \times 10^{10} \text{s}^{-1}$. Similar as for large scale sources,
medium sized sources can be considered impractical for some applications, e.g. those
that require a portable or mobile source, given their size as well as power and radiation
shielding requirements.

1.1.2 Compact Sources

In the context of fast neutron imaging, small, point-like radioisotope neutron sources
such as the spontaneous fissioning isotope $^{252}\text{Cf}$ or mixtures between an $\alpha$-emitter and
a light element using the $(\alpha, n)$-reaction are not handy. These sources show typically
a low neutron output and have a polychromatic neutron spectrum with a high gamma
radiation background that poses challenges for non-gamma blind detectors, e.g. plastic
scintillators developed in Adams et al. [40]. Furthermore, radioisotope sources cannot
be turned off, meaning that they have to be shielded and handled carefully even when
the imaging system is not running and while being transported.

Neutron generators are sources that can be turned off. Commonly and in this work, the
term neutron generator refers to a fusion-based, small scale neutron source. Contrary to
larger scale neutron sources, neutron generators can be made much less costly, are usually
compact, less complex, and produce a quasi-monoenergetic (fast) neutron spectrum. On
top of that, the proliferation risk is greatly reduced compared to research reactors and
there is no production of (high-level) radioactive waste.

A thorough overview of (compact) neutron generators and their applications is given by
Csikai [41]. Commonly, compact fast neutron generators use the deuterium-deuterium
Chapter 1. Introduction

Reaction  | $Q$-value [MeV] | Neutron energy (center of mass) [MeV]
--- | --- | ---
$^2\text{H} + ^2\text{H} \rightarrow ^3\text{He} + n$ (D-D) | 3.27 | 2.45
$^2\text{H} + ^3\text{H} \rightarrow ^4\text{He} + n$ (D-T) | 17.59 | 14.1

Table 1.1: Common nuclear reactions for compact fast neutron generators

Compact fast neutron generators commonly use the D-D and D-T nuclear reaction to produce fast neutrons. Details on these two reaction are found in Table 1.1.

Since the reactions have positive $Q$-values, the corresponding neutron source can be built compact with an electrostatically driven accelerator setup and at operating high electrostatic potentials of around 80 to 150 kV. This corresponds to an accelerating energy in the order of 80 to 150 keV for a mono-atomic particle beam. In this accelerating energy range, the total reaction cross section of the D-T fusion reaction is around two orders of magnitude larger than the corresponding one from the D-D fusion reaction (see Figure 1.2). On top of that, the D-D nuclear reaction cannot only result in the production of a neutron, but can result with a nearly equal probability in the production of a proton and one triton, which is not usable for neutron imaging. The tritium produced in the D-D nuclear reaction requires suitable radiation monitoring and handling of exhaust gas if the vacuum system is actively pumped, whereby the produced activities are usually low. While neutron sources that use either the D-D or the D-T nuclear reaction to produce fast neutrons require radiation protection material, the use of tritium for a D-T type neutron source severely increases complexity when handling, operating, and licensing such a neutron generator due to the presence of radioactive material in the target. On top of that, the higher center of mass neutron energy of around 14.1 MeV from the D-T reaction compared to the 2.45 MeV from the D-D reaction can be a challenge in detection of the higher energy neutrons or be unattractive for activation analysis applications [42]. For both the D-D and the D-T reactions, the neutrons produced in the respective neutron generator show a nearly monoenergetic spectrum for low accelerating voltages (in the order of $10^2$ keV). Still, the neutron energy is a function of the emission angle with respect to the incoming deuteron (see Figure 1.6 for the case of a D-D neutron generator). This is of interest for applications where a white neutron spectrum is unwanted, e.g. when different, distinct neutron energies are used to highlight elemental contrast in imaging applications [43], for cross section measurements [44], or when beam hardening is an undesired effect.

There are a variety of neutron generators with different designs for imaging applications, both custom, application-tailored sources and commercial ones. Typically these
Figure 1.2: Total reaction cross section of the D-D and D-T nuclear reaction

The typical deuteron energy range of 80 to 150 keV for compact fast neutron generators is shaded in green. Note that the y-scale on the left is for the D-T cross section in barn, whereas the one on the right for the D-D cross section is in $10^{-3}$ barn. Data taken from Brown et al. [45].

commercial neutron generators can suffer from a large emitting spot (in the forward direction, most relevant for imaging applications) with effective emitting spot sizes of up to a few tens of millimeter which makes them impractical for imaging applications. Chichester et al. [46] compared three commercial, hermetically-sealed, compact, portable D-T neutron sources (MP 320, P 325, and API 120) manufactured by Thermo Electron [47]. These systems were lightweight (12 to 32 kg) and had neutron yields of around $1 \times 10^8 \text{s}^{-1}$ for accelerating potentials of 95 to 110 kV and ion beam currents of 60 to 100 µA. Applications included assaying of nuclear wastes, detection of explosives or fissile materials, and bulk material analyses. No direct information on the emitting spot size was given, but for the API 120 was claimed to be less than 2 mm. Cremer et al. [48] used a D-D neutron generator (“DD-109”) with a reported neutron yield of $1 \times 10^9 \text{s}^{-1}$ from Adelphi Technology Inc. [49] to image hydrogen bearing materials. The system achieved an overall imaging resolution of 2.5 mm. Zuber [50, 51] performed neutron radiographic inspections of munitions and weapon systems using a high flux, medium sized D-D neutron source from Phoenix Nuclear Labs LLC [52] and a smaller neutron source from Starfire Industries LLC [53]. Zuber found that the former source had a nominal neutron yield of around 2 to $4 \times 10^{10} \text{s}^{-1}$ for a maximum beam current of 30 mA and a maximum accelerating potential of 300 kV. The neutron emitting spot in the gas target was a line source of neutrons with a diameter of around 1 cm in which the neutrons slowed down over a distance of around 70 cm [54]. The neutron source from Starfire
Industries LLC showed a nominal neutron yield of around $2 \times 10^9 \text{s}^{-1}$ for a maximum accelerating potential of 200 kV and a maximum beam current of 37.5 mA. The emitting spot size was not given, but Starfire Industries LLC detailed a spot size for their neutron source for neutron radiography ("nGen 800") in the order of 1 cm in their advertisement [55]. Bergaoui et al. [56] used a $1 \times 10^{10} \text{s}^{-1}$ D-D neutron generator with an effective emitting spot size of around 2 to 3 cm to investigate different collimator designs for the application of neutron radiography. Andersson et al. [57] investigated the application of fast neutron tomography on a static, large-scale nuclear fuel bundle test loop using a scaled D-T neutron generator with a neutron output of around $1 \times 10^8 \text{s}^{-1}$ manufactured by EADS Sodern [58]. When imaging with a neutron emission angle of 90° with respect to the accelerating beam the effective spot size could be reduced. However, resolution in this case was dominated by the oversimplified detector system.

Apart from spatial resolution, the interplay of the parameters source strength, emitting spot size (or volume), detector dimensions, and overall imaging geometry (e.g. sample to source distance) are relevant for (neutron) imaging. Since fast neutrons are highly penetrating, it is challenging to produce fast neutron detectors which are efficient enough to achieve reasonable exposure times in practical imaging scenarios. When increasing the thickness of such detectors, the efficiency increases, but so does the inherent blur which limits spatial resolution. However, imaging blur is also affected by the emitting spot size and the geometry of the imaging setup. Minimization of the emitting spot size decreases the source-induced blur, but can lead to an unwanted decrease in source strength under certain conditions (e.g. temperature limits in electrostatically driven accelerator setups to produce neutrons). At the same time, a small emitting spot allows for a smaller overall setup which utilizes a higher fraction of the emitted flux, as the setup can be arranged in a fan- or cone-beam imaging geometry. This allows to work with a short distance between source and imaging object. Because the neutron flux is inversely proportional to the distance squared, a lower source strength can be accepted in these configurations. Moreover, the magnification effect from a small imaging object to source distance can help increasing the spatial resolution. That all being said, a neutron source with a higher output can also achieve reasonable spatial resolution, e.g. when using a parallel-beam imaging setup, as long as the detector has an appropriately small pixel size. For large sample to source and detector to source distances, the spatial resolution can be high and under the assumption of a high neutron flux at the detector, exposure times can be reasonable.

The estimation that assumes a typical imaging scenario for a compact D-D fast neutron generator in a one-dimensional setting (see Figure 1.3) has the following constraints:
1. Minimum source to object ($d_{so}$), source to detector, and object to detector ($d_{od}$) distance: 100 mm.

2. Maximum source to detector ($d_{so} + d_{od}$) distance: 10 000 mm.

3. Minimum field of view: 200 mm.

4. Total detector size ($L_d$): 1000 mm.

5. Detector resolution ($B_d$): 0.8 mm.

6. Overall resolution ($B_o$): 1.2 mm.

7. Detector efficiency: 5 %.

8. Required flat field counts per pixel for one image: 3000.

9. Neutron output bias factor (D-D neutron source) in imaging direction: 1.4 (neutron output relative to the average output over $4\pi$).

10. Maximum allowed imaging time: 100 min.

With these constraints the analysis uses basic formulas summarized by Endrizzi [4] to compute the radiographic imaging time for different neutron outputs and emitting spot sizes. Because the image at the detector plane covers a larger area than at the object plane, the magnification, $M_{ag}$, is defined as:

$$M_{ag} = \frac{d_{so} + d_{od}}{d_{so}} \quad (1.2)$$
The image blur induced by the finite emitting spot scaled in the object plane, $B_{fo}$, can be estimated by:

$$B_{fo} = f_s \frac{M_{ag} - 1}{M_{ag}},$$  \hspace{1cm} (1.3)

where $f_s$ is the full-width at half maximum (FWHM) of the assumed Gaussian shaped emitting spot.

The image blur induced by the detector scaled to the object plane, $B_{do}$, is estimated respectively by:

$$B_{do} = \frac{B_d}{M_{ag}}$$  \hspace{1cm} (1.4)

Hence the total overall resolution at the object plane, $B_o$, can be approximated by:

$$B_o = \sqrt{B_{fo}^2 + B_{do}^2}$$  \hspace{1cm} (1.5)

For any possible geometries that satisfy those constraints outlined above the effective imaging time is estimated for one pair of emitting spot size and neutron output in Figure 1.4.

In each case, the minimal effective imaging time per radiograph is taken for any geometry that does not violate the constraints of the estimation (e.g. object to detector distance below 100 mm or overall resolution above 1.2 mm). Neutron output and emitting spot size values for typical commercially available sources were either directly taken or estimated from data published by the vendors on their website, although it should be noted that these claims were mostly not externally verified or peer-reviewed [49, 58, 53, 52, 47]. The area in the lower right has a time per radiograph below $10^{-3}$ min and is excluded from the Figure only for visual reasons to make better use of the available color range. This estimation illustrates that for one setup with a lower neutron output, but a smaller emitting spot size, the effective imaging time can be the same as for a setup with a higher neutron output, but larger emitting spot size (given the constraints outlined above). In other words, neutron output alone does not give a complete indication of how well a given neutron source will perform in an imaging application.
Figure 1.4: Time per radiograph for a range of neutron outputs (D-D) and emitting spot sizes

For the constraints on the estimation see text. The area in the upper left violates these constraints and the area in the lower right with times per radiograph well below $10^{-3}$ min is excluded to better use the available color range. The area enclosed with a dashed frame depicts typical values of emitting spot sizes and neutron outputs for commercial sources. Those values were directly taken or estimated from various vendor websites [49, 58, 53, 52, 47].

1.2 Generation I Compact D-D Neutron Generator at PSI

A compact D-D fast neutron generator has been developed at the Paul Scherrer Institute (PSI) in collaboration with the Swiss Federal Institute of Technology (ETH) with neutron imaging as its main intended use. For the context of this work, this neutron generator is labelled “Generation I” or “Gen. I”. Its small emitting spot size of around 2 mm has been a distinct design feature to keep source-induced imaging blur low and was thoroughly investigated using simulations and experiments in Zboray et al. [59] and in Adams et al. [60]. A corresponding fast neutron tomography-based imaging system using this neutron generator with an array of 88 plastic scintillator detectors was designed in Adams et al. [61], achieving exposure times in the order of hours per reconstructed image. Aside of the small emitting spot, the design of the D-D neutron generator system allowed for the placement of the imaging object close to the source. This increases the solid angle subtended by the object and increases the usable neutron flux which in turn decreases exposure time per reconstructed tomograph. The tomography system is sketched in Figure 1.5.

The D-D neutron generator housed a radio-frequency (RF) driven ion source at ground potential that was flanged onto a T-shaped borosilicate vacuum chamber, forming a right
Figure 1.5: Schematics of the compact D-D fast neutron generator tomography system at PSI

The system was developed in Adams et al. [61] (Generation I) viewed from the side. The most important components are labelled and the sensitive imaging area seen by the detector is indicated.

angle between the ion source centerline and the centerline along the long part of the vacuum chamber. Vacuum at levels of around $10^{-5}$ mbar during operation was maintained using a turbomolecular pump (TM 520 supplied by Pfeiffer Vacuum AG, Switzerland). Inside the quartz ion source chamber a deuterium plasma was kept at a pressure of around $10^{-2}$ mbar using a flat spiral antenna pressed against the back side of the glass. The RF antenna was supplied with typically 600 W of power at 13.56 MHz using an RF power supply from Advanced Energy Industries Inc. (1000 W type Cesar 1310). Reflected power was manually reduced using a changeable custom-built impedance matching circuit. A ring of 16 NdFeB permanent magnets (type NB023-42NM) was placed around the ion source chamber in a so-called multicusp arrangement to confine primary electrons by reflecting them back into the plasma [62]. Positive deuterium ions were extracted from the plasma meniscus using a pulsed extraction electrode and were accelerated in an electric potential field which was created by biasing a titanium rod to a high negative potential. The extraction pulser (Rup-3-5aN manufactured by GBS-Elektronik GmbH, Germany) had a maximum high voltage output of $-5$ kV and the high voltage power supply (SR-150-N-300 supplied by Technix, France) had a maximum high voltage output of $-150$ kV at 2 mA current. Deuterium ions hitting the target loaded the initially deuterium-free, pure titanium target with deuterium and then later initiated the D-D fusion reaction when reacting with already-implanted deuterium atoms. The D-D neutron generator achieved an estimated total neutron output of around $3 \times 10^{-6}$ s$^{-1}$ [63]. Increasing the ion accelerating voltage did not result in an expected increase in
the neutron yield. Target overheating and consequent outgassing of deuterium from the target was named as the root cause for this phenomenon, which is widely observed in the literature, e.g. in Verbeke [64] or in Kim et al. [65]. Breynat et al. [66] and later Barschall [67] detailed the critical temperature at which the deuterium dissociates and outgasses from the target for deuterium in titanium to 240°C. In the work of Adams [40] the target of the Gen. I neutron generator changed from a 12.7 mm diameter solid copper target rod to an internally actively cooled (first air and then later water) copper target rod. In those cases, a titanium cap was screwed onto the threaded end of the copper rod. With cooling, there was a significant (around a factor of five) increase in neutron output compared to the operation without cooling. The latest stage of target design (shown in Figure 2.1) was a 12.7 mm diameter pure titanium, (deionized) water-cooled beam target before the efforts outlined in this work began. Further details on the development, design efforts, and operating parameters during first fast neutron tomography tests can be found in the work of Adams [40].

For a D-D neutron generator, the typical neutron energy and relative yield distribution is outlined in Figure 1.6 versus the emission angle. This emission angle is the direction of the emitted neutron relative to the direction of the incoming deuteron that impinges on the beam target inducing the nuclear reaction. The angular neutron energy distribution $E_n(\theta)$ is found by mass and momentum conservation of the two body D-D nuclear reaction, as outlined in various works in the literature, e.g. in Csikai [41], Chichester [35], or Soubelet et al. [68]:

\[
(E_n(\theta))^{1/2} = \frac{(m_Dm_nE_D)^{1/2} \cos [\theta]}{m_{He} + m_n} + \frac{\left( m_Dm_nE_D\cos [\theta] \right)^2 + (m_{He} + m_n) [m_{He}Q + (m_{He} - m_D) E_D]^{1/2}}{m_{He} + m_n}, \tag{1.6}
\]

where $m_D$, $m_n$, and $m_{He}$ are the deuteron, neutron, and $^3$He mass, respectively, $E_D$ is the energy of the incoming deuteron, and $Q$ is the $Q$-value of the D-D fusion reaction.

The relative neutron yield (normalized to the yield at 90°) can be estimated using an expansion in Legendre polynomials of the data reported by Liskien and Paulsen [69] and a least-squares fit to the data as performed by Csikai [41]:

\[
\frac{R(\theta)}{R(90^\circ)} = A_0 + \sum_{i=1}^{n} A_i \cdot (\cos [\theta])^i, \tag{1.7}
\]
where $A_0, A_1, ..., A_n$ are the reported coefficients of the polynomials and $\theta$ is the emission angle. Soubelet [43] identified and proposed a correction to a polynomial fit error in the coefficients of the polynomials in Csikai [41]. The proposed correction is adopted in this work. Equation 1.7 was developed for deuteron energies between 50 and 500 keV.

![Deuteron energy and yield distribution](image)

(a) For a higher deuteron energy, the spread between forward (0°) and backward (180°) increases.

(b) The neutron yield relative to 90° is peaked in forward (0°) and backward (180°) direction. The two extrema of the relative yield increase with increasing deuteron energy.

Figure 1.6: Neutron energy and yield distribution

Neutron energy and relative yield distribution as a function of emission angle for a D-D neutron generator in the laboratory frame. The Figures assume only mono-atomic deuterium ions. Data taken from Liskien and Paulsen [69]. Note the different y axis ranges.

When a deuteron strikes the target, it can either undergo a fusion reaction when hitting a suitable reaction partner, or slow down and become implanted without undergoing a nuclear reaction. While slowing down, a fusion reaction can still occur, but with increasing depth into the target due to the lower energy of the deuteron, the probability of a fusion event occurring (see the cross section in Figure 1.2) has decreased and so will the neutron yield. Additionally, the deuterium ion beam can be comprised of heavier ion species, which results in a shared (lower) energy of the individual constituent atoms compared to the mono-atomic case. The energy of each atom can be approximated as a fraction of the accelerating potential energy that is inversely proportional to the ratio of its mass to the total mass of the molecule [35]. For example, for a molecular deuterium ion accelerated to 100 keV, each of the two deuteron atoms hits the target with an energy of 50 keV. This again results in a lower than expected neutron yield for a given accelerating potential. For an RF ion source, the mono-atomic ion fraction depends on the RF power, pressure in the plasma chamber, ion source wall materials, and ion source geometry [70]. For the RF ion source used in this work, a similar ion source was investigated by Wu et al. [62] who found a fraction of mono-atomic ions of more than 90%. Aside of composition of the deuterium ion beam, the deuterium density profile inside the target influences the neutron yield. Soubelet et al. [68] gave
an overview over the influence of different assumed deuterium density profiles inside the target on the neutron spectrum. Zboray et al. [59] assessed that for this D-D neutron generator, the theoretical neutron yield per second and milliampere beam current (using Equation 1.8) for a uniform deuterium distribution in a drive-in titanium target is larger compared to a non-uniform one that assumed the deuterons are concentrated around the implantation depth (around 1 µm for an accelerating potential of 100 kV). In a drive-in target configuration, the deuterium is continuously supplied to the target by the ion beam and the target does not have to be manufactured preloaded with deuterium.

Using a thick-target yield estimation, the theoretical total neutron output, \( Y \), of a neutron generator can be estimated for a mono-atomic ion beam with accelerating energy \( E_D \) from Csikai [41]:

\[
Y = \int_0^{E_D} \Phi_{\text{beam}}(E(x)) \frac{N_D(x(E)) \cdot \sigma(E)}{dE/dx} dE,
\]

(1.8)

where \( \Phi_{\text{beam}}(E(x)) \) is the deuteron flux in the target in cm\(^{-2}\) s\(^{-1}\) that depends on the ion beam current and is decreasing the further into the target the ions travel while being slowed down, \( N_D \) is the number density of deuterons in the target in cm\(^{-3}\) that is also a function of location inside the target, \( \sigma(E) \) in cm\(^2\) is the D-D fusion cross section and \( dE/dx \) is the stopping power in the target in eV cm\(^{-1}\). Stopping power values to estimate the neutron yield in this work were obtained by the SRIM (Stopping Power and Range of Ions in Matter) package [71].

### 1.3 Motivation and Scope of this Work

The inherent low neutron output of compact D-D fast neutron generators motivates the efforts undergone in this work. For applications that require a low-cost and small sized (fast) neutron source, a D-D neutron generator is a very attractive option. However, for some applications the low neutron output of these devices makes them impractical, e.g. requiring significant exposure times for neutron imaging in the order of a few hours. For practical applications the exposure time should be in the order of tens of minutes to make fast neutron generators a viable option. Other, non-imaging related techniques such as cross section measurements [44] or elemental-sensitive investigation techniques [43] will also benefit from an increase in neutron output. An important benefit (besides an increase in output) of a higher accelerating potential of a D-D neutron generator is a broader energy range of the emitted neutrons, as shown in Figure 1.6a. Limiting factors of neutron output of the compact D-D neutron generator used in this work were
outgassing of deuterium from the beam target due to thermal constraints and high voltage breakdowns preventing higher accelerating voltages.

The problem of outgassing of implanted deuterium from the drive-in titanium target is addressed in Chapter 2, where the thermal analysis, design, construction, and testing of a rotating copper rod that was thinly coated with titanium is presented. In Chapter 3 a detailed characterization of the total neutron output and the emitting spot size, both of which are among the key parameters for the D-D neutron generator system for the use of neutron tomography, is developed using simulations and experimental techniques. A next iteration ("Generation II" or "Gen. II") of the compact D-D fast neutron generator is described in Chapter 4. The developments of new system included changes to the vacuum chamber, the ion extraction system, the use of an electron suppression electrode, and the switch from an RF-driven to a microwave-driven ion source. These changes are motivated, justified with simulations, and experimental results are discussed.
Effective cooling is of paramount importance for the stable operation of any target that is irradiated with an energetic ion beam. Since almost all of the impinging ions energy is deposited as heat in the target, the neutron generation rate is limited by the maximum heat load on the target before the metal hydride formed by implanting deuterium in the host material dissociates (i.e., deuterium outgasses from the target).

Titanium (Ti) is a widely chosen material for the target of a neutron generator because it favours a high deuterium storage capability with D:Ti ratios of up to 2:1 [72]. Furthermore, it is a relatively low-Z material which means the stopping power of the host material is a smaller fraction of the combined stopping power than it would be with a high-Z material of the same atomic ratio [73]. The major limitation of titanium is the aforementioned and widely reported outgassing of implanted deuterium from the target in case of overheating, which occurs at around 230 to 250°C [66, 67]. A detailed review of the temperature limitation of titanium as a hydrogen occluding material is presented in Zboray et al. [59]. In the absence of target overheating, the higher the accelerating voltage or the higher the ion beam current, the higher is the neutron output of a neutron generator (due to the cross section dependence, see Figure 1.2). Yet, both influence the beam power density on the target which in turn affects the target temperature that must remain below the outgassing limit. Otherwise, the deuterium density in the target decreases and the expected gain in neutron output is averted. Thus, a higher power density requires better heat removal from the target which motivates a thorough investigation of the ion beam target design.

The target of a compact fast neutron generator is typically cooled with a chilled fluid flowing on the back side of the target. In the context of D-D or D-T neutron generators
several target constructions have been developed to allow a higher beam power density on the target. Jung et al. [74] numerically analysed the temperature of a fixed planar titanium drive-in target. Their analysis for a 760 W deuterium beam (95 keV, 8 mA) with a beam spot size on the target of around 13.5 mm showed that the maximum temperature on the target was well above the level of thermic disintegration of titanium hydride. Reijonen [75] and Ludewigt et al. [76] mounted the fixed target in a conical configuration, aiming to spread the heat flux of the impinging energetic ion beam over a larger area (3 mm in diameter, 50 mm of beam-swept depth). The drawback of this approach is that the spreading of the ion beam on the target increases the neutron emitting spot size in at least one dimension.

Another way of increasing the effective target surface is to use an oscillating beam by vibrating or rotating the target. A rotating target provides the possibility to increase the beam power, source strength, and target life up to an order of magnitude for a large-scale D-T neutron source [77]. Several large scale D-T neutron generators employ a rotating target as summarized for example in Booth et al. [78] or Peto and Pepelnik [77] and references therein. Song et al. [79] proposed a rotating tritium target system for a D-T neutron generator. Their computational fluid dynamics (CFD) simulations showed that big coolant layer thickness, big coolant flow rate, and high rotating speed enhanced the cooling of the target system. However, the effects of the coolant layer thickness and flow rate on the heat transfer were found to be very small. Vala et al. [80] performed and evaluated CFD simulations for a medium sized D-T neutron generator with a rotating target disk. Following their simulations, they designed and tested a water-cooled rotating tritium loaded target holder.

The above highlighted importance of source to object distance and large solid angle for neutron imaging application motivates a thorough investigation of the heat transfer analysis, design, and experimental performance of a rotating target rod system for a compact D-D neutron generator with the application of fast neutron imaging. In this work the heat transfer of a rotating copper target rod coated with titanium is investigated using COMSOL Multiphysics 5.4 [81]. The goal is to allow for a larger beam power density on the target spot to increase the total neutron output, while preventing deuterium outgassing, and therefore reducing exposure times for imaging applications. Most of the below presented results have been published in Kromer et al. [82].
Chapter 2. Rotating Target for Generation I Neutron Generator

2.1 Target Design Considerations

As mentioned earlier, various researchers have reported a drop of the neutron yield of a D-D neutron generator over time and attributed this to target overheating and consequent outgassing of deuterium from the target. Apart of exceeding the local target temperature beyond the critical temperature at which the hydrogen in the target dissociates and outgasses, in principle a drop in neutron yield can also be attributed to (after Peto and Pepelnik [77]):

1. Sputtering by the energetic ions which reduces the target thickness.

2. Oxygen ions in the beam can form an oxide layer on the target surface, whose presence strongly reduces the density of target nuclei at the surface by detrapping the deuterium ions or retarding the migration of target nuclei into the surface region [83, 84, 85, 86].

3. Burning out of deuterium by the D-D reaction, especially important for sealed neutron sources. This is of minor concern for a drive-in D-D neutron generator as the deuterium density in the target is replenished by the ion beam. It is mentioned for completeness and will not be addressed further.

The design of any target for a D-D neutron generator should be optimized with respect to these phenomena. The oxide layer on the target surface can form either by contribution of oxygen in the residual gas of the vacuum chamber or from impurities in the plasma ion source. It would in principle be possible to determine the latter by analysing the mass spectra of the ion beam. Such a measurement was not carried out in the current work. Using a 13.56 MHz RF ion source which is comparable to the ion source used in this work Wu [87] investigated the mass spectra of a hydrogen ion beam with a Faraday cup. The ratio between impurities and atomic hydrogen ions was less than 10%. It is though questionable to which extent this finding can be transferred to the deuterium ion source used in the present work. Therefore, the question of the origin of the observed oxide layer remains open.

The majority of the D-D and D-T neutron generators use a solid metal as the target material because a metallic target can easily be biased to a negative or positive potential allowing the acceleration of the ions towards the target. Gillich et al. [73] investigated the performance of a plastic target (CD$_2$). While the theoretical yield of such a target is higher than that of a metal hydride target, experiments revealed that the plastic target degrades over the course of an experiment. Nonetheless, it remains an interesting option for further exploration, e.g. by using a circular foil target that gets frequently
replenished automatically. A gaseous target eliminates the problem of overheating but poses challenges on practical design. Also, achieving a small neutron emitting spot size is typically not possible since the low stopping power of a gaseous target results in a large spatial spread of the emitting spot size in one dimension (e.g. for the gas target in Kulcinski et al. [54] the emitting spot had a diameter of around 1 cm in which the deuterons slowed down over a distance of around 70 cm). Moreover, a gaseous target requires differential pumping which does increase complexity and overall size of the neutron source. For solid targets, titanium is commonly used as the target material in a neutron generator due to its capability of holding a higher density of hydrogen in comparison with other metals forming hydrides as target materials such as erbium, zirconium, or scandium [73]. While for example scandium hydride is expected to be thermodynamically more stable than titanium at high temperatures [64], keeping the titanium hydride target at a moderate temperature seems to be more promising due to the higher hydrogen storage capability of titanium [66] and the lower stopping power of titanium hydride which in turn leads to a higher neutron yield [73].

One major drawback of titanium is its low thermal conductivity of around 20 W m$^{-1}$ K$^{-1}$ [88]. Hence the adopted solution is to coat the outer surface of a material that has a high thermal conductivity such as molybdenum or copper with titanium, as done in Reijonen et al. [89], Ludewigt et al. [76], Song et al. [79], and Vala et al. [80]. This makes use of the high hydrogen storage capability of titanium and the high heat removal rate of the backing material. When assessing the thickness of the titanium coating a trade-off has to be made between the target lifetime and the target surface temperature. The lifetime of the target is limited due to the sputtering of the target material. A thicker target will result in both a higher lifetime but also in a higher target temperature due to the low thermal conductivity of titanium. The trade-off on the overall target thickness is further affected by the attenuation of the neutrons when they pass through the target. Copper is chosen as the target backing material due to its suitability under high vacuum conditions as well as its high thermal conductivity compared to other metals. CuCrZr (copper-chromium-zirconium) and CuOFE (oxygen-free high conductivity copper) copper alloys are considered in this study. The alloys differ in their thermal conductivity, 300 W m$^{-1}$ K for the former and 390 W m$^{-1}$ K for the latter at 20$^\circ$C [90]. CuCrZr favours a higher mechanical strength but apart of the higher thermal conductivity CuOFE is more applicable in high vacuum conditions due to its high purity.

While rotating, the target will be subjected to a repeating cycle of a rapid temperature rise as it rotates through the beam, a rapid quench as the heat is conducted to the backing material and a gradual cooling as the target rotates around to the beam spot again [91]. Results presented in Song et al. [79] indicate that a higher rotational speed will effectively reduce the target temperature. However, a high rotational velocity poses
practical difficulties. The unit, e.g. a motor, driving the rotating of the target has to be either biased to high voltage or be electrically insulated. Moreover, the rotating target must not break the vacuum inside the vacuum chamber and coolant lines have to be prevented from twisting.

The thickness of the chilled water flowing on the back of the target affects both the heat removal rate and the neutron attenuation. The coolant flow rate will influence the flow distribution and in turn the heat removal rate. The target rod that was used in the Gen. I D-D neutron generator at PSI as described in Adams et al. [40] is made of pure titanium. It consists of two titanium pipes, where the coolant flows downwards the target on the inside of the inner pipe and vertically upwards in an annulus shaped by the outer and inner pipe. The inner pipes outer diameter is 6.35 mm and the outer pipe has an outer diameter of 12.7 mm. Both pipes have a wall thickness of 0.5 mm. See Figure 2.1 for a cut view of the neutron generator extraction system. To keep the core benefits of the neutron generator setup (small source to object distance and large access to neutrons in the forward direction) the new rotating target rod should have a similar arrangement of pipes to form the coolant channel.

![Figure 2.1: Cut view of the pure titanium beam target](image)

Cut view of the pure titanium beam target used in the Gen. I D-D neutron generator system at PSI. Deuterium ion paths and titanium wall thickness not to scale.

The constraints on the target design are presented in Table 2.1. The outer diameter is the maximum diameter which fits in the vacuum chamber of the Gen. I D-D neutron
Chapter 2. Rotating Target for Generation I Neutron Generator

degenerator [40]. Deionized water is employed as the coolant and circulated with a recirculation chiller from ThermoFischer (ThermoFlex 1400 Recirculating Chiller) with a nominal volumetric flow rate at the outlet of \(12.5 \text{L min}^{-1}\) at 4.1 bar. An off the shelf hollow shaft magnetic rotary feedthrough (Part Number 14400) is supplied by VacSol GmbH, Germany, and the rotation of the coolant lines is arranged with a mechanical two-channel rotary union (MP2001-C) from COSMAU Technology Co., Ltd, China. The maximum ion beam power of 300 W is specified by a high voltage power supply (SR-150-N-300 from Technix, France) which can afford at most a voltage of \(-150 \text{kV}\) and a maximum current of 2 mA. Titanium is adopted as the hydrogen occluding material for the above mentioned reasons.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value / Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer diameter</td>
<td>40 mm</td>
</tr>
<tr>
<td>Cooling</td>
<td>Deionized water in a recirculation chiller</td>
</tr>
<tr>
<td>Coolant dynamic seal</td>
<td>Mechanical two-channel rotary union</td>
</tr>
<tr>
<td>Vacuum dynamic seal</td>
<td>Magnetic rotary feedthrough</td>
</tr>
<tr>
<td>Neutron emitting spot size</td>
<td>2 mm ([59, 60])</td>
</tr>
<tr>
<td>Maximum ion beam power</td>
<td>300 W (150 kV, 2 mA)</td>
</tr>
<tr>
<td>Maximum beam power density</td>
<td>9.55 kW cm(^{-2}) (300 W, 2 mm)</td>
</tr>
<tr>
<td>Target material</td>
<td>Titanium coated on copper</td>
</tr>
</tbody>
</table>

Table 2.1: Design constraints and choices for the rotating rod drive

Design constraints and choices for the rotating rod drive in the target system of a D-D neutron generator.

2.2 Conjugate Heat Transfer Simulation

CFD simulations with COMSOL Multiphysics 5.4 \([81]\) were carried out to study the heat transfer of a rotating rod target system assuming single-phase steady-state conditions. This Section introduces the model chosen in the simulations, informs about the mesh as well as associated mesh refinement study, and shows the results for the conjugate heat transfer analysis for various selected parameters.

A three-dimensional (3D) model was chosen for the investigation where the basic design concept is shown in Figure 2.2 following the considerations in Table 2.1. Copper was identified as the backing material to enhance heat removal from the target. The coolant channels were arranged in coaxial rings formed by thin-walled copper tubes. The inside of the target was filled with ambient air. This approach was chosen to limit unwanted neutron attenuation by the target structure and because the heat transfer in layers beneath the coolant outflow channel has insignificant impact on the target surface.
temperature. In the simplified target model used in the simulations, only the titanium, copper, and coolant outflow channel were included. The total length of the simplified target domain was fixed to 200 mm and the ion beam was hitting the target outer surface at 100 mm from the fluid inlet.

![CAD cross section view of the target model](image)

**Figure 2.2: CAD cross section view of the target model**

CAD view of the real target model in A and simplified geometry used in the simulations in B. Note that the titanium layer is scaled up. Figure adapted from Kromer et al. [82].

### 2.2.1 Model

The ion beam spot is far away from the bottom cap of the target rod. Since the fluid flow in the simplified model was assumed to be fully developed, it must be identified at what distance downstream the point where the fluid flows from the inner channel into the outer channel the fluid can be considered fully developed. The result of a two-dimensional (2D) axisymmetric study with a target outer diameter of 40 mm, 3 mm copper backing layer, 2 mm coolant channels, and 1 mm inner wall thickness for a water volumetric flow rate of 3 L min\(^{-1}\) with a laminar flow interface is shown in Figure 2.3. The results show that for a distance of around 40 mm downstream the flow obstacle, the fluid flow can be considered fully developed. Hence the conclusions following this simulation study in this work are only valid under the assumption that this minimal distance is kept.

A 3D conjugate heat transfer problem was set up which solved for conservation of energy, mass, and momentum in the fluid and for conservation of energy in the solid parts.
Chapter 2. Rotating Target for Generation I Neutron Generator

(a) Fluid flow with velocity magnitude. (b) Velocity magnitude differences at various axial locations relative to $z_0 = 175$ mm. The dashed lines are the wall-fluid interface.

Figure 2.3: Justification of using a simplified geometry in CFD simulations

Since the fluid flow is already fully developed after around 40 mm beyond the point where fluid flows from the inner annulus in the outer one, a simplified geometry was used.

The boundary conditions for the fluid interface were:

1. The fluid flow was in single-phase and steady-state.
2. The coolant (water) inlet velocity was computed at atmospheric pressure from the measured volumetric flow rate of $3 \text{ L min}^{-1}$. Unless otherwise mentioned, all results in this work were obtained with a volumetric flow rate of $3 \text{ L min}^{-1}$. As an initial step in the simulation, the radial profile of the coolant inlet velocity was computed in a 2D simulation of the fluid channel. This velocity distribution was then mapped to the 3D simulation as the inlet velocity.
3. A laminar flow interface was chosen in COMSOL for cases where the Reynolds number was below 4000. Only for one study a low Reynolds $k$-ε interface was chosen which is explicitly mentioned during the parameter study that follows in this work.

The boundary conditions for the heat transfer interface were:

1. The coolant inlet temperature and the initial values for the temperature in the solid parts were set to 20 °C.
2. The deuterium ion beam was modelled with a Gaussian cross section. It was striking the target perpendicular to its surface at 100 mm from the inlet with a full
width at half maximum (FWHM) of 2 mm, which was based on prior simulations and experiments of this neutron generator [59, 60]. COMSOL took the curvature of the target surface into account when computing the beam profile at the target surface.

3. The rotation of the target rod around the symmetry axis was modelled by adding a translational motion term to the heat transfer interface of the solid parts. COMSOL processed this by adding a convective term in the energy equations of the solid parts. The velocity field in this term was adjusted according to the set rotational velocity of the target similar to other works on this topic [79, 80].

4. Outgassing of deuterium from the titanium host material was considered to occur at 240°C in the context of this work.

5. The standard Non-Isothermal Flow interface that COMSOL offers for conjugate heat transfer was used to couple fluid properties and temperature.

Other material related boundary conditions were:

1. The thickness of the titanium layer was chosen to be 5 µm, which was a compromise between maximum surface temperature and target lifetime due to sputtering.

2. Two copper alloys were considered, CuOFE and CuCrZr. The former is a high purity, oxygen-free alloy with a slightly higher thermal conductivity, whereas CuCrZr was considered due to its superior mechanical properties and widespread availability.

2.2.2 Mesh

The mesh in the 2D axisymmetric study was made out of rectangular elements and only the fluid part was meshed. To achieve convergence the region closer to the wall and the region towards the inlet were more refined. The mesh in the 3D study is displayed in Figure 2.4. It consisted of hexahedral mesh elements in both solid and fluid part. The solid part contained three mesh nodes in radial direction. First the inlet boundary face was meshed and swept through the whole domain. The number of mesh elements per unit length increased towards the center of the domain where the modelled ion beam power impinged onto the outer target surface. The number of mesh nodes has been optimized with respect to convergence and computational cost.

A mesh refinement study proved independence of the fluid properties for laminar flow and target outer surface temperature on the mesh. In this study a coarse, normal, and fine mesh as shown in Figure 2.5 was set up.
In all studies the beam power was set to 300 W and the rotational velocity of the target was 200 rpm. Coolant channel thickness was 2 mm and the copper layer had a thickness of 3 mm. The mesh in $x$ direction was refined in the same proportion as shown for the solid and fluid part. The mesh refinement was not repeated for the low Reynolds $k$-$\epsilon$ model since the shear layer near the wall was already accurately captured as shown in Figure 2.6.

<table>
<thead>
<tr>
<th>Mesh identifier</th>
<th>Mesh elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>A (coarse)</td>
<td>420 000</td>
</tr>
<tr>
<td>B (normal)</td>
<td>1 776 000</td>
</tr>
<tr>
<td>C (fine)</td>
<td>3 080 000</td>
</tr>
</tbody>
</table>

Table 2.2: Number of mesh elements for the conjugate heat transfer simulation
The temperature and velocity magnitude distribution in $z$ direction into the target at the position where the beam impinged on the target is shown in Figure 2.7a and Figure 2.7b, respectively. Figure 2.8a and Figure 2.8b show the relative differences between the coarse and normal mesh with respect to the fine mesh. As can be seen the relative differences between the three meshes are insignificant. Table 2.2 summarizes the number of mesh elements. The final mesh was chosen with 756 000 mesh elements in the fluid domain and 126 000 mesh elements in the solid domain.

Figure 2.6: Distance of the cell center from the wall-fluid interface
In order to use the low Reynolds $k$-$\epsilon$ interface in COMSOL, the dimensionless distance to cell center has to be less than 0.5 which is true for the mesh used in this work.

Figure 2.7: Mesh refinement using temperature and velocity magnitude
Mesh refinement study investigating temperature and velocity magnitudes in mesh A, B, and C at the beamspot in $z$ direction. The dashed lines are the wall-fluid interface. Note the different $x$ ranges and $y$ scales.
Figure 2.8: Effect of the mesh size on temperature and velocity profiles

The result of the mesh refinement study is presented as temperature and velocity magnitude differences between mesh A and B relative to mesh C. The dashed lines are the wall-fluid interface. Note the different $x$ ranges and $y$ scales.
2.2.3 Analysis

2.2.3.1 Validation of Single-Phase Flow Assumption

As outlined earlier the conjugate heat transfer assumed single-phase flow conditions. In Figure 2.9 the two worst case combinations of model parameters investigated in this work are presented. Both studies were performed with a coolant channel thickness of 1.5 mm, a rotational velocity of 25 rpm, and a total beam power density of 9.55 kW cm\(^{-2}\) which corresponds to 300 W on a 2 mm beam spot. The CuCrZr thickness was set to 1 mm and 3 mm, respectively. In the case of the 1 mm thickness, the assumption of single-phase flow is not validated, since the temperature of the wall-fluid interface was around 220 °C. This corresponds to the worst case combination of model parameters investigated in this work (high beam power, low copper thickness, lower thermal conductivity, low rotational velocity, low coolant flow rate). The next worst case combination was the one with the 3 mm copper layer. In this study, the wall-fluid interface had a temperature of around 75 °C which means that the assumption of single-phase flow is valid. From this one can conclude that for all studied cases with a CuCrZr (or CuOFE) thickness larger than 1 mm, the assumption of single-phase flow holds.

![Temperature profiles for different copper backing thicknesses](image)

**Figure 2.9: Temperature profiles for different copper backing thicknesses**

The copper wall temperature (dashed lines) was below the boiling point of water for a copper backing thicknesses above 1 mm. In the presented study the rotational velocity was 25 rpm and the ion beam power was 300 W. Figure adapted from Kromer et al. [82].
2.2.3.2 Copper Material and Thickness

The influence of the copper backing layer thickness on the maximum target surface temperature is shown in Figure 2.10. In these studies the total beam power density was set to 6.47 kW cm\(^{-2}\) which corresponds to a total beam power of 200 W. The target rotational velocity was 25 rpm and the coolant layer thickness varied between 1.5 mm and 7 mm. The value for the total beam power was chosen because results at this beam power indicated that the influence of other parameters such as the target rotational velocity had a greater impact on heat removal compared to the other parameters. Computational cost could be reduced in comparing the less influential parameters at a lower beam power setting. However, for preselected parameters, cross validations show that the trends observed at this beam power setting of 200 W are comparable to those at 300 W total beam power. From the results in Figure 2.10 one can conclude that for both CuCrZr and CuOFE, the larger the backing layer thickness, the lower is the maximum target temperature. It is important to keep in mind that the single-phase flow assumption was not valid for the simulations with the 1 mm copper thickness. In cases with CuOFE as the backing material, the maximum target temperature was around 15 to 20% lower compared to the cases with CuCrZr as the backing material.

Figure 2.10: Maximum target temperatures as function of the copper thickness

For both CuCrZr and CuOFE the larger the backing layer thickness, the lower the maximum target surface temperature. The total beam power in these studies was set to 200 W. Figure adapted from Kromer et al. [82].
The copper backing thickness, made out of CuOFE, was proposed to be 3 mm. Beyond a copper thickness of 3 mm, the incremental decrease in maximum target surface temperature becomes less for an increase in the copper layer thickness.

### 2.2.3.3 Coolant Layer Thickness

Rearranging the data from Figure 2.10 one can visualize the influence of the water layer thickness on the maximum target surface temperature in Figure 2.11. The model parameters are the same as those in Figure 2.10. For both CuCrZr and CuOFE the variation in the maximum target temperature with an increase in coolant channel thickness is smaller. On top of that, the coolant layer thickness has insignificant impact on the maximum target temperature. This finding agrees well with results in Song et al. [79].

![Figure 2.11: Maximum target temperature as function of the coolant layer thickness](image)

For both CuCrZr and CuOFE coolant layer thickness has insignificant impact on the maximum target temperature. The total beam power in these studies was set to 200 W.

The coolant layer thickness was proposed to be 2 mm. A larger coolant layer thickness would not decrease the maximum target surface temperature by much, but increase the parasitic neutron attenuation by the target as investigated later in Section 2.3.2.
2.2.3.4 Coolant Flow Rate

The effect of the increase of the coolant mass flow rate on the maximum target temperature is depicted in Figure 2.12 for four investigated volumetric flow rates. If the velocity magnitude of the fluid in the channel becomes large enough, turbulent flow can occur. This greatly enhances heat transfer and will lead to a lower target temperature. For the volumetric flow rates of 3 L min\(^{-1}\) to 20 L min\(^{-1}\) that were investigated in this study the Reynolds number in the coolant channel center ranges from 1000 to 6700. Those cases with a volumetric flow rate of 12 L min\(^{-1}\) and 20 L min\(^{-1}\) were computed with the low Reynolds k-\(\epsilon\) turbulent model. For all presented studies the copper was CuOFE with a thickness of 3 mm, a coolant channel thickness of 2.675 mm (coolant channel thickness in the previous target design), a target rotational velocity of 25 rpm and a beam power density of 6.47 kW cm\(^{-2}\) (200 W on a 2 mm beam spot). The results show that an increase in the coolant flow rate by a factor of around six decreases the maximum target temperature only by around 4%. Keeping in mind the computational cost and effects of the coolant flow rate combined with the effect of the thickness of the coolant layer on the maximum target surface temperature, the investigation was not repeated for the final coolant layer thickness (2 mm) chosen in this work.

![Figure 2.12: Influence of the coolant flow rate on the maximum target temperature](image)

The maximum target temperature decreases insignificantly with an increase in the coolant volumetric flow rate. The total beam power in these studies was set to 200 W. Figure adapted from Kromer et al. [82].
The coolant flow rate was proposed to be kept at 3 L min$^{-1}$. Larger coolant flow rates would not decrease the maximum target surface temperature much but require a redesign of the existing cooling system and associated equipment of the neutron generator.

### 2.2.3.5 Rotational Velocity

The rotational velocity of the target has a significant impact on the maximum target surface temperature as shown in Figure 2.13. In this study the CuOFE thickness was set to 3 mm, the water coolant layer thickness is 2 mm at a volumetric flow rate of 3 L min$^{-1}$. The total beam power density was set to 9.55 kW cm$^{-2}$, which corresponds to the largest beam power (300 W) achievable with the existing high voltage power supply of the neutron generator for the 2 mm beam spot. Figure 2.13 shows that controlling the rotational velocity allows to reduce the maximum target temperature well below the outgassing limit. In Song et al. [79] this is explained with a lower heat accumulation followed by an increase in uniformity of the temperature distribution around the target when the rotational velocity increases.

![Figure 2.13: Decrease of the target temperature with increasing rotational velocity of the target](image)

The total beam power in these studies was set to 300 W. Figure adapted from Kromer et al. [82].

A motor and target driving system was designed to exceed a rotational velocity of the target rod of 100 rpm.
2.2.3.6 Beam Power Density

To summarize, the above conjugate heat transfer analysis concluded that a target rod with an outer diameter of 40 mm made out of CuOFE with a thickness of 3 mm, a titanium layer thickness of 5 µm, a coolant channel thickness of 2 mm with a 3 L min$^{-1}$ coolant flow rate, and a target rotational velocity that exceeds 100 rpm resulted in a target temperature well below the outgassing limit. At the same time this configuration kept parasitic attenuation of direct 2.8 MeV neutrons emitted under an angle of 0° with respect to the incoming deuterium ion beam by the target low at around 35% (see details in Section 2.3.2). Expected beam power densities that could be achieved within the neutron generator system ranged between 1.9 and 2.8 kW cm$^{-2}$ (corresponding to 60 to 90 W total beam power). In the context of this work, upgrades of the neutron generator system will not allow the total beam power to exceed a maximal value of 300 W (9.55 kW cm$^{-2}$ on a 2 mm beam spot). Results of a simulation shown in Figure 2.14 for a target rotational velocity of 220 rpm for these beam power densities estimate that the maximum target surface temperature will be at most at around 160°C. This is well below the outgassing limit of deuterium in titanium (around 240°C).

Figure 2.14: CFD results of the maximum target temperature

CFD results of the maximum target temperature for three different beam power densities at a target rotational velocity of 220 rpm. A: 2.55 kW cm$^{-2}$ (70 W total beam power), B: 6.47 kW cm$^{-2}$ (200 W total beam power), and C: 9.55 kW cm$^{-2}$ (300 W total beam power). For all settings, the maximum target surface temperature remains well below the outgassing temperature of deuterium in titanium (240°C). Figure adapted from Kromer et al. [82].

2.3 Mechanical Design

The above outlined conjugate heat transfer analysis resulted in a proposed target design for a 40 mm diameter target rod with a 5 µm thick titanium layer, a 3 mm thick copper
layer of type CuOFE, and a 2 mm thick coolant outflow channel. As mentioned above, the inner structure of the target was not included in the the conjugate heat transfer analysis. Yet, the amount of material (water and piping structure) inside the target is to be kept as low as reasonably possible for the sake of parasitic neutron attenuation. A sketch in Figure 2.15 shows the extraction system in a cross section view of the proposed target structure installed into the neutron generator system.

![Figure 2.15: Cross section view of the proposed target structure around the extraction region](image)

Titanium coating not included. Deuterium ion paths and quartz chamber wall thickness not to scale.

Apart of heat transfer considerations the lifetime limitation of the target in terms of loss of titanium layer due to sputtering when the ion beam hits the target was examined. Also, it is validated that the parasitic attenuation of neutrons in the target is low in the final, proposed target configuration. Finally, the support structure that holds the new target rod is presented.

### 2.3.1 Sputtering of Titanium

The impinging deuterium ions are slowed down in the target primarily by electronic stopping. As they slow down recoils begin to contribute and dominate the energy loss. Recoils occurring in the surface region might sputter off titanium atoms if the energy
of the titanium atom exceeds the surface binding energy of the target. The amount of sputtered target atoms per incident ion was found using the software package Stopping and Ranges of Ions in Matter (SRIM, [71]). It should be noted that the surface binding energies are difficult to determine and their value will change as the target roughens after initial sputtering [71]. The sputtering yield, $R_{Ti}$, of titanium with a surface binding energy of 4.9 eV for 100 keV deuterium ions is determined from SRIM to $R_{Ti} = 0.00176 \ \text{atoms ions}^{-1}$. The simulation contained 99 999 simulated 100 keV deuterium ion histories that hit a pure titanium target of 5 µm thickness at 0° incidence angle.

The sputter rate $S_c$ in cm s$^{-1}$ of a surface layer with compound c due to ion bombardment can be estimated from Hsieh et al. [92]:

$$S_c = \frac{M \ R_c \ j_{\text{beam}}}{\rho \ N_A \ e}, \ (2.1)$$

where $M$ is the molar weight of the target in g mol$^{-1}$, $R_c$ is the sputtering yield for the compound c in atoms ions$^{-1}$, $j_{\text{beam}}$ is the bombarding ion beam current density in A cm$^{-2}$, $\rho$ is the target density in g cm$^{-3}$, $N_A$ is the Avogadro constant in mol$^{-1}$, and $e$ is the electron charge in C. Taking the ion beam diameter as 2 mm and the ion beam current to 1 mA, Equation 2.1 yields a sputter rate of $S_{Ti} = 6.17 \times 10^{-9}$ cm s$^{-1}$. This allows the estimation of the average target lifetime — with respect to complete loss of the titanium layer — under the assumptions that the sputtering is uniform over the whole 2 mm beam spot and the aforementioned constraints from SRIM.

The effect of a target rotation on the average lifetime, $t_{\text{dep}}$, in seconds can be estimated by the increase in the effective beam area on the target due to its rotation:

$$t_{\text{dep}} = \frac{d_{\text{target}}}{\pi \ d_{\text{beam}} \ S_c}, \ (2.2)$$

where $d_{\text{target}}$ is the target thickness in cm, $d_{\text{beam}}$ is the ion beam diameter in cm, $d_{\text{rod}}$ is the target rod outer diameter in cm, and $S_c$ is the sputter rate in cm s$^{-1}$. Using the previously obtained value for $S_{Ti}$, a 2 mm beam spot, and a 40 mm diameter target rod in Equation 2.2 yields a lifetime of around 1800 h for a titanium layer thickness of 5 µm. This already long target lifetime limitation is eliminated by the target holder design and coating a larger area of the target with titanium (see Section 2.3.3). The target holding system allows to insert the rod either deeper down or further up into the vacuum.
chamber. This means a different (titanium coated) target region can be exposed to the ion beam.

2.3.2 Attenuation of Neutrons by the Target

Under the assumption that the Beer-Lambert law [93] (see Equation 1.1) holds and neglecting the influence of the air inside the target, the fraction of neutrons in the forward direction attenuated by the target is estimated from:

\[
1 - \frac{I}{I_0} = 1 - \left( \exp \left[ -\mu_{\text{water}} d_{\text{water}} \right] \exp \left[ -\mu_{\text{Cu}} d_{\text{Cu}} \right] \exp \left[ -\mu_{\text{Ti}} d_{\text{Ti}} \right] \right),
\]  

(2.3)

where \( I \) is the attenuated neutron intensity, \( I_0 \) denotes the unattenuated neutron beam, \( \mu \) is the (averaged) neutron attenuation coefficient, and \( d_i \) is the total thickness of the respective material \( i \) that the beam passes through in the target. The material properties for titanium, copper, and water are summarized in Table 2.3. The total microscopic cross sections for neutrons between 2 and 3 MeV for the estimation of the averaged neutron attenuation coefficient are taken from the ENDF/B-VII.1 [94] database.

<table>
<thead>
<tr>
<th>Material</th>
<th>Composition</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Titanium</td>
<td>Ti-46 (8.25%), Ti-47 (7.44%), Ti-48 (73.72%),</td>
<td>4.506 g cm(^{-3})</td>
</tr>
<tr>
<td></td>
<td>Ti-49 (5.41%), Ti-50 (5.18%)</td>
<td></td>
</tr>
<tr>
<td>Copper</td>
<td>Cu-63 (69.15%), Cu-65 (30.85%)</td>
<td>8.960 g cm(^{-3})</td>
</tr>
<tr>
<td>Water</td>
<td>H-1 (2), O-16 (1)</td>
<td>1.000 g cm(^{-3})</td>
</tr>
</tbody>
</table>

Table 2.3: Material parameters for the estimation of the fast neutron attenuation by the proposed target

Values taken from Rumble [1].

The total microscopic cross sections from the ENDF/B-VII.1 database are averaged in the energy interval \([E_0, E_1] = [2, 3]\) MeV:

\[
\sigma_{\text{avg}} = \int_{E_0}^{E_1} \sigma(E)dE \quad \frac{E_1 - E_0}{E_1 - E_0}
\]
Chapter 2. Rotating Target for Generation I Neutron Generator

Then, the estimated averaged attenuation coefficients can be calculated from:

$$\mu_{avg} = \frac{N_A \rho \sigma_{avg}}{M},$$

where $N_A$ is the Avogadro constant in mol$^{-1}$, $\rho$ the density of the compound in g cm$^{-3}$, and $M$ its molar mass in g mol$^{-1}$. This results in $\mu_{Ti} = 0.20$ cm$^{-1}$, $\mu_{Cu} = 0.27$ cm$^{-1}$, and $\mu_{water} = 0.20$ cm$^{-1}$. Results of the fraction of attenuated neutrons in the target for selected ranges and combinations of the compound thicknesses $d_i$ are presented in Figure 2.17. The Figure displays the total thicknesses that the neutron beam has to pass in a straight line through the target, i.e. twice the thickness of CuOFE, four times the water column, four times the inner pipe wall, and two times the titanium layer as can be inferred from Figure 2.16.

**Figure 2.16: Schematics of the target to explain the study of unwanted neutron attenuation in the target**

The attenuation in the target was estimated assuming a neutron beam that propagates along the dashed line through the target. Dimensions not to scale.

For the proposed target configuration, 35% of 2 to 3 MeV neutrons are attenuated by the target. Increasing the CuOFE thickness by 1 mm will decrease the maximum surface target temperature only by around 3% (see Figure 2.10), but increase the fraction of attenuated neutrons by around the same amount. Keeping in mind the aforementioned larger target temperature reduction effect of increasing the rotational velocity of the target compared to the CuOFE thickness, the increase in CuOFE thickness is not justified. The reduction of the maximum target temperature with an increase in water layer thickness was even less significant (see Figure 2.11) with a comparable effect on the fraction of attenuation neutrons as with the CuOFE. Finally, as long as the structural integrity of the target can be maintained, the inner copper pipes should be as thin as possible.
Chapter 2. Rotating Target for Generation I Neutron Generator

Figure 2.17: Estimation of the fraction of neutrons attenuated in the target for various target material thicknesses

Estimation of the fraction of direct neutrons (2 to 3 MeV) attenuated in the target for various target material thicknesses. Both CuOFE and the pipes are made out of “copper” as defined in Table 2.3. The proposed target configuration is indicated in red with a parasitic attenuation of direct neutrons of around 35%.

Tests in a pressure chamber have shown that the 1 mm CuCrZr pipes can withstand a pressure gradient of at least 6 bar which meant that the pipe thickness was fixed at 1 mm as the deionized water recirculating chiller operated at a pressure of 4.1 bar.

2.3.3 Mechanical Assembly

The rotating target rod sketched in Figure 2.2 was designed and manufactured in two parts, an upper and a lower one. The outer layer of the parts that are exposed to the vacuum system of the neutron generator are made out of CuOFE. The lower part can be screwed into the upper part allowing for leak tight insertion into the vacuum chamber. The upper part contained all the inner target structures that form the inlet and outlet channels. These structures were made out of CuCrZr due to its superior mechanical
properties and its lower price compared to CuOFE. The lower part of the target was a tube with an outer diameter of 40 mm, 3 mm wall thickness, and a length of 400 mm. A spherical bottom cap was welded onto the tube on its lower end. Figure 2.18 shows a cross section cut view of this lower part. Since the ion beam impinged only on this lower part, merely the entire lower part (and not the upper section of the target rod) was coated thinly with grade 2 titanium. The coating was performed by swiss-PVD coating AG, Switzerland, who estimated the thickness of the coating to be 4.8 µm in the region where the ion beam hits the target surface.

![Figure 2.18: Cross section cut view of the lower, coated part of the proposed target](image)

The manufacturer estimated the titanium coating thickness to be 4.8 µm around the spot where the deuterium beam hits the target. Optical microscopy estimated the thickness at the upper edge to 2.9 to 3.6 µm.

Around 10 mm of the target tube at the end where the lower part is screwed onto the upper part were cut off to evaluate the coating thickness. Three optical microscopy measurements estimated the thickness of the coating there to be between 2.9 to 3.6 µm. One of these microscopy results is shown in Figures 2.19, the other two are included in the Appendix A in Figure A.1 and A.2. This concludes that the titanium layer thickness at the point where the deuterium ion beam was designed to hit the target was at least 2.9 µm. This is likely a very conservative estimate, because the manufacturer designed the process of coating so that the thickness near the beam target region approached the desired 5 µm.

To allow for a rotating target rod biased at a negative high voltage, all components for the drive rotating the target also had to be biased to negative high voltage. Therefore, an aluminum support structure was built that included a pneumatic motor, a two-channel rotary union, a hollow magnetic ferrofluidic rotary vacuum feedthrough, and the drive system to connect the motor rod to the target as shown in Figure 2.20. This structure was hanging from the ceiling that houses the neutron generator and was isolated using epoxy resin insulators supplied by BINAME bvba, Belgium.
Figure 2.19: Optical microscopy measurements of the titanium coating thickness
Samples were taken far away from the beam spot at the upper edge of the lower part of the target.

Figure 2.20: Target support structure and rotating mechanism
The aluminum rotating target support structure was hanging from the ceiling and housed the pneumatic motor, a two-channel rotary union, as well as a magnetic ferrofluidic vacuum seal. Figure adapted from Kromer et al. [82].
Chapter 2. Rotating Target for Generation I Neutron Generator

A corona ring below the aluminum support structure reduced the risk of high voltage breakdowns between the high voltage terminal and the grounded Faraday cage of the neutron generator. The pneumatic motor LRD-R-300/280 was supplied by Reiss GmbH & Co. KG, Germany, and the hollow ferrofluidic vacuum feedthrough was supplied by VacSol GmbH, Germany. Since the target was biased to a negative high voltage, the water used in the recirculating chiller was deionized. Several two-channel rotary unions from different vendors and of different material compositions (MP2001-C from COSMAU, China, LTM-2121 as well as GSP-120 from DSTI Inc., USA) were installed in the system. However, all of them have failed after between 1 to 2 weeks of operation (around 8 h of operation per day) when the rotary sealings were terminally rusted. The manufacturer DSTI Inc. attributed this failure mode to the combination of a low remaining conductivity of the deionized water in combination with the high voltage applied to the whole target rod drive structure. After reviewing the beam powers that are expected in the near-term to be reached within the neutron generator, the cooling fluid was changed to pressured air at the same pressure as the formerly used deionized water (4.1 bar). No deterioration of the target performance (i.e. outgassing of deuterium) was observed after the change in coolant fluid.

2.4 Performance of the Rotating Target

2.4.1 Loading of the Fresh Target

After assembly and installation of the new target rod into the neutron generator system, the fresh, “deuterium-free” titanium had to be loaded with deuterium. Loading was performed with high voltage settings of around $-40$ to $-60$ kV and an averaged target current of 0.7 to 1.5 mA read by the instrument of the high voltage supply. This relatively low target current was chosen to reduce the number of high voltage sparks at around 0.1 sparks per minute and high duty factor of the extraction electrode pulsing. The latter setting increased the deuterium ion beam current that enhanced the rate of deuterium implantation in the target. Other operational conditions were a rotational velocity of the target rod of around 220 rpm, 600 W RF power, and a pressure of $3 \times 10^{-2}$ mbar in the ion source indicated by a PKR 251 Compact Full Range Gauge supplied by Pfeiffer Vacuum, Switzerland. The extraction electrode was biased to $-3$ kV with a pulsing frequency of 3 kHz at a maximum duty factor of around 90%. After the plasma in the ion source was ignited, a high voltage and duty factor setting was found so that the neutron generator operated at a low number of high voltage breakdowns and was kept at this level for around 3 to 7 h per operating day. Figure 2.21 shows one such typical loading cycle, where the neutron yield is estimated by correlating a Monte Carlo
simulation (MCNP6, [95]) model and the averaged ambient dose rate measured with an LB6411 neutron probe [96] as detailed in Section 3.1.

![Graph showing neutron yield over time](image)

**Figure 2.21: Typical loading process of the fresh rotating target**

At 100 min the operation was interrupted for reasons unrelated to the neutron source performance. The high voltage settings ranged from −40 to −60 kV. Figure adapted from Kromer et al. [82].

The loading procedure was followed until the neutron yield reached a plateau after around 20 h of loading spread over a few days. At this point the target was considered fully loaded. The loading time with the novel, rotating target is considerably longer compared to the formerly used, static target. This is attributed to the rotation of the target, which increases the effective target surface that is exposed to the deuterium ion beam.

### 2.4.2 Comparison between Rotating and Stationary Target

Visual inspection of the target after a cumulative operation of around 100 h did not reveal any rainbow-shaded coloration seen in the past with the former, pure titanium target as compared in the photographs in Figure 2.22. Titanium dihydride that is forming when the deuterium is implanted in the titanium matrix has a reported greyish color [97], hence the rainbow-shaded coloration seen in the former, non-rotating target indicated extreme overheating and oxidation.

The temperature inside and on the surface of the target rod was not measured, but this visual check suggested that target overheating did not occur with the novel, rotating target at the beam powers where the neutron generator was operating at. Repeated inspections after longer operation of the new target rod at elevated power levels of
Figure 2.22: Photographs of the ion beam spot on the non-rotating, pure titanium target rod (A) and on the novel, rotating one (B)

The rainbow-shaded coloration indicated extreme overheating and oxidation with the former target that was not observed with rotating target after around 100 h of cumulative operation. The two images are approximately to scale. For the determination of the neutron emitting spot size see Section 3.2.

around $-90\,\text{kV}$ and 1.0 to 1.5 mA showed only the expected dark metallic coloration of the region where the ion beam strikes the target and not the rainbow-shaded coloration that would indicate overheating.

The highest total neutron yield averaged over the entire pulsed extraction duty cycle during the initial testing was estimated to $4.8 \times 10^7 \, \text{s}^{-1}$ for a high voltage setting of $-107\,\text{kV}$ and an averaged target current of 0.9 mA. The neutron output was estimated using the technique described in Section 3.1. However, high voltage breakdowns between the high voltage terminal and the grounded Faraday cage limited stable operation with no more than 1 spark per couple of minutes to around $-80$ to $-90\,\text{kV}$. This limitation was overcome in a later stage of this project as outlined in Chapter 4. At stable operating conditions, the total averaged neutron yield per unit beam power against the beam power is shown in Figure 2.23. With increase in beam power, the neutron yield increases as expected which implies no loss of deuterium implantation density, which confirms the visual observation that outgassing did not take place. The neutron output per unit of beam power with the previously used, static, pure titanium target estimated in Adams et al. [60] dropped when the beam power was increased beyond around 40 W. In this experiment the duty factor of the extraction electrode pulsing was 12\%, the high voltage was biased at $-60$ to $-120\,\text{kV}$, and the averaged target current was between 0.15 and 0.5 mA.
The estimation indicated that the target was not overheating with increasing power. Data from Adams et al. [60] was recorded at 12% duty factor of extraction and −60 to −120 kV high voltage.

The ratio between total estimated averaged neutron yield (labelled as “actual” yield) and the theoretical yield for a fully loaded, ideal, TiD$_2$ target with uniform deuterium density calculated from Equation 1.8 is shown in Figure 2.24. Details on this thick-target yield estimation can be found in Csikai [41]. In comparison to findings in Adams et al. [60], where the same ratio as shown in Figure 2.24 was investigated for a non-rotating, pure titanium target, the ratio does not decrease when the beam power increases. This indicates that overheating did not take place and that deuterium was not outgassing with the novel, rotating target. The offset between actual and theoretical yield might be attributed to the unknown deuterium density profile inside the target, a D:Ti ratio less than 2:1, as well as uncertainties in the MCNP6 model and the LB6411 neutron probe characteristics. Additionally, beam losses when the ion beam is neutralized in the gap between extraction electrode and target are not captured by the theoretical yield assessment. Moreover, when computing the beam power from the averaged target current read by the high voltage power supply, the superposition of the unknown leakage current on the current reading overestimates the actual beam current. This leakage current can be from the deionized water coolant lines or electrons liberated from the target in the sputtering process. The instrument of the high voltage power supply read a target current in the order of 0.01 mA when the RF plasma ion source was turned off and hence without ion beam present. However, electromagnetic interferences in devices near the neutron generator when the RF power supply was turned on have been a reoccurring challenge. It is probable that the RF field also interferes with the reading of the instrument of the high voltage power supply. Upgrades to the neutron source in a later stage of this project included the switch to a microwave ion source which allowed...
confinement of the microwave radiation inside the waveguide, for details see Section 4.2.

![Figure 2.24: Ratio between actual and theoretical neutron yield](image)

The ratio indicates no loss of deuterium from the target due to outgassing. Data from Adams et al. [60] was recorded at 12\% duty factor of extraction and −60 to −120 kV high voltage.

A direct comparison between the previously used, static, pure titanium target and the novel, rotating target made with titanium coated on copper designed in this work is shown in Figure 2.25. In both cases the respective targets were operating at their stable operating condition, which is limited by high voltage breakdowns and considered as “less than one spark per couple of minutes”. Typically, the total neutron yield estimated in the case of the static, pure titanium target was around $6.6 \times 10^6$ s$^{-1}$. For the novel, rotating target, the typical neutron yield was estimated to around $2.9 \times 10^7$ s$^{-1}$. Moreover, it was possible to operate the neutron generator with the rotating target at a significantly higher beam power level at almost a factor of three higher than compared with the static target. The static, pure titanium target has experienced significant overheating and outgassing as shown in Figure 2.22 and discussed in detail in Adams et al. [60].
Figure 2.25: Gained enhancement of the neutron yield with the rotating target compared to the static target

Figure adapted from Kromer et al. [82].
Chapter 3

Development of Source Characterization Techniques

The main characteristics of interest of a compact fast D-D neutron generator important for imaging applications are the overall neutron output and the emitting spot size. There are various techniques reported in the literature with varying degree of fidelity to measure the total neutron output of a neutron generator. Sometimes, the neutron yield of a custom-tailored source is given only as a design value, e.g. to outline the potential of the source, and no detailed explanation is given how this figure was obtained, for example in Chichester et al. [46], Vala et al. [80], or Huang et al. [98]. The challenge is that if not handled carefully, the neutron output can be significantly over- or underestimated. One of the techniques to measure the neutron yield is using a neutron detector and comparing the experimental measurements to simulations with Monte Carlo calculation codes. Bergaoui et al. [99] compared measurements with a neutron dosimeter and a $^3$He neutron detector to Monte Carlo simulations where they assumed a V-shaped neutron spatial distribution and an isotropic 2.45 MeV (D-D) neutron source. Other techniques involve measurements only with a neutron detector and using transformation or anisotropic factors to estimate the total neutron output, as done for example by Das et al. [100] who measured the neutron count rate in a detector and considered a solid angle transformation factor. However, details on why this specific value for the factor was chosen to estimate the neutron yield is not given in their work. A similar, but experimental method is to perform activation analyses in combination with anisotropy corrections. Wu et al. [101] measured the neutron yield using the activation of circular gold foils and compared the measurements with other neutron sources with a known yield. Ayllon et al. [42] used indium as irradiation sample to estimate the neutron flux for their High Flux D-D Neutron Generator. They included Monte Carlo simulations to characterize the neutron energy distribution at the sample holder location where the
object for their experiment would be placed. Another common method to determine
the total neutron output is the presentation of simulation results alone, as done for ex-
ample in Song et al. [79] that estimated the neutron output of their neutron generator
by simulating the neutron flux with a Monte Carlo method at distinct locations around
the neutron source.

As outlined in Section 1.2, to make use of the intrinsic small neutron output of compact
D-D neutron generators, a close source to sample distance should be chosen to maximize
the available output solid angle in imaging applications. This enables imaging in a fan-
or cone-beam arrangement, given that the neutron emitting spot size is small enough
to have a low source-induced blur in the images. Hence the size of the emitting spot
is a very important parameter of a compact neutron generator considered for neutron
imaging applications. In the literature, for applications where the exact knowledge of
the emitting spot size is of minor importance, the emitting spot size is sometimes not
explicitly given, or no explanations of how it was estimated are presented [80, 98]. There
are different techniques for (compact) neutron generators to determine the emitting spot
size. In Jung et al. [74] the deuterium ion beam current profile for a D-D neutron gen-
erator was directly measured using a single slit and a Faraday cup. For voltages lower
than the typical operation setting when the neutron generator was running, the beam
profile was determined to be Gaussian shaped. This technique cannot be adopted for
the neutron generator in this work because of the short distance between target (at high
voltage) and ion source (at ground potential), which makes installation of a Faraday
cup difficult and can create unwanted high voltage breakdowns. Furthermore, measur-
ing the profile at low voltages does not necessarily generalize well to higher, typical
operating voltages as the value of the electric potential field influences the beam pro-
file. Long et al. [102] switched the usual beam target with a high purity silicon target
and bombarded it with deuterium ions. Post irradiation analysis of the target using
secondary ion mass spectrometry was done to estimate the ion beam profile. Measure-
ments with a scintillation screen inside the vacuum chamber and a CCD camera were
performed in Wang et al. [103]. The requirement for this to work is that the ion source
must be biased to the accelerating potential (since the target was removed). For the
neutron source in this work, that would require complicated isolation of the ion source
RF generator. On top of that, the space inside the vacuum chamber is limited and a
viewport cannot be installed without a complete replacement of the borosilicate vacuum
chamber. All these techniques to measure the ion beam profile to estimate the emitting
spot size, although successful, share one significant disadvantage: the ion beam spatial
distribution does not have to be representative of the emitting spot size spatial distrib-
ution. Because the underlying assumption in this case would be that the distribution
of implanted deuterium in the target has to reflect the ion beam spatial distribution.
Not only can there be heterogeneity in deuterium loading of the fresh, deuterium-free, drive-in titanium target. There can be diffusion of deuterium away from the surface of the target, where the deuterium is implanted at depths of around 1 µm [59] into the target, even after loading was completed.

In this work, the neutron output was estimated by developing a technique that combines the response of a Berthold LB6411 neutron probe [96] with a detailed MCNP6 Monte Carlo model [95]. The emitting spot size was determined using an attenuating edge technique, in which a tungsten piece is moved stepwise perpendicular to the direct path of neutrons between emitting spot and a custom-made neutron detector. Charged particle tracing simulations with COMSOL Multiphysics were carried out to compare the experimentally found emitting spot size with the deuterium ion distribution on the target. In the following Section, the MCNP6 model and the experimental technique are carefully described and benchmarking results from COMSOL Multiphysics are presented. Some of these results have been submitted for publication in Kromer et al. [104].

### 3.1 Neutron Output

The neutron output in this work was estimated combining the ambient dose reading of an LB6411 neutron probe with correct scatter-correction using a detailed Monte Carlo model with the simulation code MCNP6. In the model, the neutron flux per simulated source particle was determined at distinct locations around the neutron source. The cells in which the neutron flux was estimated were spherical with a diameter that corresponded to the diameter of the experimental neutron probe itself, 25 cm. From the manufacturer of the neutron probe the neutron fluence response \( R(e) \) in counts per fluence, where fluence was neutrons per cm\(^2\), was known. The MCNP6 model estimated the averaged neutron flux \( T(e) \) in one energy bin \( e \) in number of neutrons per cm\(^2\) per source particle using an F4 tally at the location of the neutron probe. The F4 tally estimates the averaged neutron flux in a MCNP6 cell in neutrons per cm\(^2\) per source particle using a track length estimator. Knowing the relationship between the count rate in the neutron probe and its ambient dose rate reading from the manufacturer of the probe allowed to estimate the total neutron yield, \( Y_{\text{exp}} \), when combining the ambient dose rate reading with the expected count rate from the MCNP6 model:

\[
Y_{\text{exp}} = \frac{k H}{p \sum_e T(e) R(e)},
\]  

(3.1)
where $p$ denotes the number of source particles set in MCNP6, the constant $k = 0.79$ given by the manufacturer was in units of counts in the neutron probe per second per µSv h$^{-1}$, and $H$ was the ambient dose rate reading in the neutron probe in µSv h$^{-1}$. This ambient dose rate recorded in the LB6411 neutron probe was read out using a Berthold LB112 stationary dose rate monitor [105]. The device was set up to output a current that was proportional to the recorded ambient dose rate. From the voltage drop across a resistor the ambient dose rate could be recorded with a frequency of around 1 Hz.

### 3.1.1 MCNP6 Model

Earlier investigations of the neutron flux around the neutron source, described in Adams et al. [63], were performed with a simple model of the neutron source and have shown that the most important components to include in the model are those structural materials that are close to the neutron source, as well as the walls, floor, and concrete ceiling that enclose the facility which housed the neutron generator. In this work, a more detailed MCNP6 model was developed with a significantly higher level of geometric complexity as presented in Figure 3.1. Figure 3.2 shows a photograph of the neutron generator to allow to compare the digital twin developed in MCNP6 with the real layout. The goal of this MCNP6 model was to develop a tool that allows a more accurate characterization of the neutron source and to quantify the gain in neutron yield achieved in various improvement stages of the neutron generator as described in Chapter 4. On top of that, the detailed model of the neutron generator and components in its vicinity served in a parallel study of developing and applying novel energy-selective imaging applications [68]. The thin-walled Faraday cage around the source was not included in the model as it was not significantly attenuating and its layout would change depending on the experimental goals of a specific day. Only about 3% of fast neutrons with an energy of 2.5 MeV are attenuated by 1 mm pure copper, and the cage was made of copper foil with a thickness of 0.3 mm. Similarly, vacuum piping, valves, and connections were omitted from the model due to their small size and consequent limited influence on the neutron flux. The aluminum structure (aluminum arc) to support an experiment to perform energy-selective transmission tomography [68] was included in the model. The movable trolley running along the arc-shaped track was omitted because its inner layout changed often and it was located at a distance of 1 m which meant it had negligible influence on the overall neutron spectrum. Other equipment, that was more than 1 m away from the neutron source was neglected because the long distance reduced the influence of these components on the neutron distribution. Furthermore, since the room that
housed the neutron source was also used for other purposes, the location of structures far away from the source generally changed in an unpredictable fashion.

(a) 3D view without F4 tallies.  
(b) Position of the F4 tallies.

**Figure 3.1:** 3D representation of the MCNP6 model  
Figure adapted from Kromer et al. [104].

**Figure 3.2:** Photograph of the neutron generator, components in its vicinity, and movable detector system  
The movable detector system is described in Soubet et al. [68]. Figure adapted from Kromer et al. [104].
Details close to the source were modelled carefully with MCNP6 and included:

- Target (titanium layer, copper backing, water coolant channels, and copper pipes)
- Vacuum chamber and ion source system (copper aperture, magnets, quartz glass ion chamber, and teflon RF antenna clamp)
- Matching network to tune the RF impedance (modelled as estimated weighted average of aluminum, air, and copper)
- Aluminum profiles, table supporting the neutron source, and rotating target support structure (modelled as estimated weighted average of aluminum and air)
- Teflon holder to clamp vacuum chamber against turbomolecular pump
- Turbomolecular pump (modelled as aluminum cylinder)
- Corona ring around rotating target support structure
- Aluminum arc structure to support moving detector setup
- Insulators to hold the rotating target support structure (modelled as epoxy cylinders)
- Electrical rack that housed various electric devices to control the neutron source (modelled as estimated weighted average of aluminum and air)
- Walls, floor, and ceiling that enclosed the room housing the neutron source

Ten F4 tallies in forward (+x), backward (−x), and side direction (±y), respectively, were used to estimate the neutron flux around the neutron generator. These F4 tallies were modelled as spheres with a diameter of 25 cm that corresponded to that diameter of the LB6411 probe used in the neutron generator facility to estimate the ambient neutron dose rate. In Figure 3.3 the model of the neutron generator is shown as seen from above and in Figure 3.4 the model is shown from the side viewing in backward (−x) direction. Note that the F4 tallies in the +y direction are shifted in +z direction compared to the ones in −y direction by 1 cm to account for the position of the aluminum arc.

The room housing the neutron generator is modelled as filled with air and all material definitions in the model used in this work are taken from McConn et al. [106]. The material details of the matching network, electrical rack, turbomolecular pump, aluminum rotating target support structure, and aluminum profiles were approximated using the estimated weighted average of their constituents, e.g. air and aluminum in the case of the aluminum profile or copper, air, and aluminum in case of the matching network.
This was done because their inner structure was very complex and modelling every detail would be both inefficient and the overall effect on the estimation of the neutron flux would be insignificant compared to other components.

![Figure 3.3: MCNP6 model of the neutron generator seen from the top](image1)

Figure 3.3: MCNP6 model of the neutron generator seen from the top

![Figure 3.4: MCNP6 model of the neutron generator seen from the side](image2)

Figure 3.4: MCNP6 model of the neutron generator seen from the side

The neutron source was modelled as a point source with an angular energy and relative yield information according to Figure 1.6 depending on the energy of the deuterium ion.
A more complex spatial source definition with a Gaussian distribution was not included in this model. During typical operation, the LB6411 neutron probe would be at least 20 cm away from the source. Hence the influence of the spatial source distribution of the around 2 mm emitting spot size on the neutron yield estimation would be negligible.

Results of the F4 flux tallies are shown in Figure 3.5. Figure 3.5a depicts the flux in the F4 tallies far from the neutron source at around 100 cm and Figure 3.5b presents the flux in tallies closer to the source. In backward direction due to the ion source and matching network, tallies are placed in a different interval compared to the other directions.

![Figure 3.5: Fast neutron flux estimated with MCNP6](image)

The flux levels estimated by the F4 tallies were lower further away from the source compared to closer by, as is expected. The angular energy yield is also reflected in the results with a peak in neutron flux at around 2.8 MeV, 2.5 MeV, and 2.2 MeV in forward, side, and backward direction, respectively. This agrees well with the expectations of the source definition. The flux peak in the side directions is not as sharp as in the other directions because the solid angle subtended by tallies in the side direction included parts of the target of the neutron generator. This means a higher fraction of neutrons starting in forward direction ($x > 0$) being scattered into the F4 tally in the sides than compared to the backward direction. This effect is more pronounced for a tally closer to the source as can also be seen in Figure 3.5.

### 3.1.2 LB6411 Neutron Probe Experiment

Two Berthold LB6411 neutron probes (also called “Bonner” spheres), labelled NP1 and NP2, were used to validate the MCNP6 model and benchmark the accuracy of the
model to estimate the neutron output. The approach was chosen that one LB6411 probe remained at a fixed location and the other one was moved around the neutron source but pointing always in the same direction towards the neutron emitting spot. Figure 3.6 illustrates the arrangement of the two probes. The fixed neutron probe, NP1, was connected to the Berthold LB112 stationary dose rate monitor that recorded the ambient dose rate read by the probe. This system provided an electric current that was proportional to the reading of the ambient dose rate. An Arduino Uno [107] sampled the voltage drop over a resistor with a frequency of 1 Hz and the signals were calibrated using the display of the LB112 dose rate monitor for a wide range of readings. The output of the moving second probe, NP2, was read with an Arduino Due-based [107] pulsed-readout system that integrated the counts in intervals of 30 s in the neutron probe. The data streams from both of these readout tracks were stored permanently in a mariDB database [108]. Figure 3.7 sketches the readout system.

After repositioning the moving sphere manually and restarting the neutron source, recording of experimental data at one NP2 position commenced after the neutron dose rate, measured in NP1, remained constant for around 10 min. In both cases, Equation 3.1 was used for an estimate of the total neutron yield. In the case of the moving
sphere NP2, the numerator of Equation 3.1 was taken as the measured counts (\(= k H\)) at that sphere’s position, since it was not connected to the ambient dose rate monitor. Figure 3.8 shows the neutron output in units of the ambient dose rate at various distances between the F4 tally cell in MCNP6 and the neutron emitting spot constituting a quick tool to estimate the neutron output based on the reading of the ambient dose rate monitor.

Figure 3.7: Diagram of the readout system during the LB6411 neutron probe experiment

Figure 3.8: Neutron output estimate relative to the ambient dose rate in the LB6411 neutron probe

During a typical operation of the neutron source, the sphere was fixed at \(y = 70\) cm. Figure adapted from Kromer et al. [104].
The idea behind the validation of the model is that at different NP2 positions the total neutron output estimated with each of the probes NP1 and NP2 should agree. Figure 3.9 shows the ratio between the neutron output estimated with the moving probe, NP2, and the fixed probe, NP1, for various distances of the moving probe. Overall, the ratio of the estimated outputs agrees within 15%, which confirms the validity of the approach outlined here to assess the neutron output. At three positions the probes where switched, i.e. the fixed NP1 became the moving one and the moving NP2 became the fixed one, to control for a bias in either LB6411 neutron probe towards their readout mode which was not found as shown in Table 3.1. The largest difference was observed when the probe was moved in the side direction to $y = -53$ cm with around 7% deviation from the output computed using the fixed sphere.

![Figure 3.9: Comparison of the estimated neutron output obtained by both LB6411 probes](image)

The observed discrepancies can originate in the MCNP6 model from the accumulation of earlier outlined simplifications (e.g. omitting of smaller components, components further away from the source) and from inaccuracies during the measurement with the LB6411 probes in finding the accurate position of NP2 in 3D. Furthermore, the internal structure of the LB6411 neutron probe was not precisely known and hence not modelled, and the constant $k$ that relates counts in the LB6411 neutron probe to ambient dose rate reading given by the manufacturer could also have introduced inaccuracies. Lastly, the RF field that generates the plasma in the ion source has been a frequent cause of interference with
measurements in the past, which could also contribute to the measurements outlined here. Independence of the orientation of the LB6411 neutron probe orientation was verified by turning the moving probe by 90° and finding no significant deviation in the count rate.

<table>
<thead>
<tr>
<th>Neutron probe</th>
<th>Position [cm]</th>
<th>Readout</th>
<th>Estimated neutron output [10^6 s⁻¹]</th>
<th>Relative difference [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NP1</td>
<td>x = 55</td>
<td>count rate</td>
<td>6.3</td>
<td></td>
</tr>
<tr>
<td>NP2</td>
<td>y = 55</td>
<td>dose</td>
<td>6.1</td>
<td>3</td>
</tr>
<tr>
<td>NP1</td>
<td>y = −53</td>
<td>count rate</td>
<td>6.2</td>
<td></td>
</tr>
<tr>
<td>NP2</td>
<td>y = 55</td>
<td>dose</td>
<td>6.7</td>
<td>7</td>
</tr>
<tr>
<td>NP1</td>
<td>x = −66</td>
<td>count rate</td>
<td>7.3</td>
<td></td>
</tr>
<tr>
<td>NP2</td>
<td>y = 55</td>
<td>dose</td>
<td>6.8</td>
<td>7</td>
</tr>
</tbody>
</table>

Table 3.1: Influence of the readout mode on the estimated neutron output

The formerly fixed probe, NP1, was the moving one and the formerly moving one, NP2, was the fixed one at y = 55 cm. There is no significant difference outside the expected variations (see Figure 3.9) in the estimated neutron output.

3.2 Emitting Spot Size

The neutron emitting spot size was estimated with an attenuating edge technique, in which a tungsten edge is moved perpendicular into the path between the emitting spot and a fast neutron detector. The response of the movement of the edge on the count rate in the detector produced a characteristic curve that was used to estimate the size of the emitting spot. Results of this experiment are compared with charged particle tracing simulations in COMSOL Multiphysics that estimated the ion beam spot size on the surface of the neutron generator target.

3.2.1 Attenuating Edge Measurements

In the context of this work the neutron emitting spot was assumed to be Gaussian shaped and the FWHM of that Gaussian shaped distribution was considered the neutron emitting spot size. Jung et al. [74] determined the ion beam current profile of their D-D neutron generator — with an RF ion source that was similar to the one used in this work — to be approximately Gaussian shaped. The experimental method outlined below to determine the neutron emitting spot size is a more refined version of the approach outlined in Adams et al. [60]. An attenuating edge was moved perpendicular into the path between the neutron emitting spot and the detector. Recording the response of
the count rate in the detector to the movement of the edge results in a characteristic curve, the so-called edge response or edge spread function (ESF) [109]. Fitting a logistic function to the ESF allows for direct evaluation of the FWHM [110]:

\[
f(x, a, b, c, d) = \frac{a}{1 + \exp\left(-\frac{x-b}{c}\right)} + d \tag{3.2}
\]

\[
\text{FWHM} = 2 \log\left(2 \sqrt{2 + 3} \right) c \tag{3.3}
\]

For an infinitely long measurement time a small detector size is desirable. However, because the measurement time during the experiment and the neutron flux are finite, the stochastic part of the uncertainty starts dominating the error in the fit to the ESF. That motivated to investigate the sensitivity of the parameters for the experimental setup with MCNP6 simulations, which is outlined in the following Section.

### 3.2.1.1 Sensitivity Study of Experimental Parameters

The fast neutron detector, developed in Adams et al. [63], consisted of a polyvinyl toluene (PVT)-based plastic scintillator and two silicon photomultipliers (SiPMs), effectively read out as if it were one SiPM and therefore referred to as if they were a single SiPM, mounted against the back side of the scintillator. In the following investigation, the term “detector” referred to the scintillator alone, as the SiPM did not directly convert the neutrons into electrical signals, but relied on the plastic scintillator for conversion of neutron energy into light. The scintillator was chosen as one readily available with dimensions of $5 \times 5 \times 20 \text{ mm}^3$ (width $\times$ height $\times$ depth, where depth is in neutron beam direction). For this plastic scintillator the efficiency is approximately 15\% for a depth of 20 mm assuming an energy cutoff of 0.7 MeV [63].

A high density tungsten alloy with more than 90\% tungsten supplied by Plansee, Switzerland, was chosen as the material of the attenuating edge piece due to its high density and comparably high neutron attenuation while still ensuring good machining properties. A high neutron attenuation coefficient was desirable because with increasing thickness the measurement becomes more problematic due to larger penumbra effect or higher sensitivity to misalignment. MCNP6 was used to find a set of selected parameters for the attenuating edge measurement. The model is outlined in a sketch in Figure 3.10, where the parameters that were investigated in the sensitivity study are colored in red.

An MCNP6 model was set up that included the target, coolant, and a simplified model of the borosilicate vacuum chamber of the neutron generator, the tungsten attenuating
edge, and the plastic scintillator. Material definitions were taken from McConn et al. [106] for target, coolant, and vacuum chamber. The attenuating edge was defined as pure tungsten, since the composition of non-tungsten elements in the alloy was unknown, yet their contribution was considered secondary. The plastic scintillator composition was modelled using the datasheet from the manufacturer [111]. The model simulated $10^5$ neutron histories originating from a disc source with a uniform emission profile (i.e. a top-hat profile) with an energy cutoff of 0.1 MeV. Neutrons were emitted in a cone covering a total angle of 2° (see Figure 3.10) with a starting energy of 2.8 MeV, corresponding to neutrons produced in the forward direction for 100 keV deuterium ions, see Figure 1.6. Separate MCNP6 models were set up for different combinations of the parameters outlined above. The attenuating edge was placed at a distance of 11.05 cm from the source which corresponded to the minimal distance that was possible due to the copper Faraday cage around the neutron generator. This Faraday cage was typically fitted around the neutron generator to limit RF induced electromagnetic interferences. The height of all the components (except for the detector, which was far away and thus subtended a small solid angle) was set so that its respective backwards face away from the source covered the solid angle of the source (2°) plus 10%. Cross-validations have shown that the number of emitted neutrons ($10^4$, $10^6$), height of components (plus 20%), and a variation in the neutron energy (2.6 MeV, 2.7 MeV, 2.9 MeV) have negligible impact on the trend of the optimization of the experimental setup. For each source disc diameter in MCNP6 100 edge positions were simulated in different MCNP6 input files. Because the position of the copper Faraday cage around the neutron generator typically changed from any one experiment to the next, the copper sheet was not included in this optimization study. The same held for the lead shield, which would be adjusted later in the experiment, so it was not included in the MCNP6 model. Since fast neutrons with an energy of 2.8 MeV are only attenuated around 3% in 1 mm copper and around 6% in
3 mm lead, this did not significantly bias the results. For each MCNP6 simulation, the total reaction rate, $R_{tot}$, inside the detector volume per source particle was computed from:

$$R_{tot} = V \int_{E_{\text{min}}}^{E_{\text{max}}} \Sigma_H(E) T(E) dE,$$

where $T(E)$ denotes the flux level estimated by an F4 tally inside the detector volume $V$, $E_{\text{max}}$ the maximum energy center bin value of the F4 tally and $E_{\text{min}}$ the minimal one, and $\Sigma_H(E)$ the (total) macroscopic cross section for hydrogen. This estimation assumes that an interaction between a neutron and the carbon in the scintillator does not contribute to the detection of a neutron given the very low light yield of this interaction as investigated in Adams et al. [63].

A geometric correction, $f$, was applied to take into account that the neutrons in the simulation were emitted only in a $2^\circ$ cone using the relative yield curve $Y(\theta) = R(\theta)/R(90^\circ)$ from Figure 1.6:

$$f = \frac{\int_1^{15} Y(\theta) d\theta}{\int_0^{180} Y(\theta) d\theta}$$

The count rate in the detector, $C$, was computed with the total emitted neutrons per second $Y$ to $C = Y f R_{tot}$. Taking the energy cutoff in the detector electronics into account to discriminate Bremsstrahlung X-ray radiation [63], the cutoff corrected count rate reads:

$$C_{\text{cutoff}} = Y \frac{\int_0^{15} Y(\beta) d\beta}{\int_0^{180} Y(\beta) d\beta} \left(1 - \frac{E_{\text{cutoff}}}{E_{\text{neutron}}}\right) V \int_{E_{\text{min}}}^{E_{\text{max}}} \Sigma_H(E) T(E) dE$$

The total number of counts in the detector, $I$, was estimated by multiplying $C_{\text{cutoff}}$ with the counting time per edge position:

$$I = C_{\text{cutoff}} \frac{t_{\text{tot}}}{N_{\text{edge}}}$$
As a basis for comparison the conditions for the variable in Table 3.2 were assumed. For one set of parameters (detector to source distance and attenuating tungsten edge thickness) the flux from the F4 tally, \( T(e) \), was extracted and the intensity of counts in the detector was computed using Equation 3.7. The corresponding ESF was then evaluated by collecting all the edge positions for one set of parameters, i.e. one geometry defined in MCNP6.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total counting time</td>
<td>( t_{\text{tot}} )</td>
<td>5 h</td>
</tr>
<tr>
<td>Number of edge positions</td>
<td>( N_{\text{edge}} )</td>
<td>100</td>
</tr>
<tr>
<td>Total neutron yield</td>
<td>( Y )</td>
<td>( 3 \times 10^7 ) s(^{-1} )</td>
</tr>
<tr>
<td>Neutron energy</td>
<td>( E_{\text{neutron}} )</td>
<td>2.8 MeV</td>
</tr>
<tr>
<td>Cutoff energy</td>
<td>( E_{\text{cutoff}} )</td>
<td>0.7 MeV</td>
</tr>
</tbody>
</table>

Table 3.2: Assumed experimental conditions for the emitting spot size measurement

To investigate the sensitivity of the geometry to stochastic variation from one simulated measurement series to the next, a repetition of the MCNP6 simulation was approximated by drawing 1000 random samples of the total number of counts, \( I \), in the detector from a Poisson distribution, at each simulated edge position and for each of the geometries. Each set of random values for one geometry and one range of edge positions corresponds to a simulated ESF measurement dataset. Fitting with a logistic function as in Equation 3.2 was applied to each normalized simulated ESF dataset. This procedure that is outlined in Figure 3.11 was followed for each set of parameters, i.e. each geometry in MCNP6. For any given geometry, the spread in terms of standard deviation in the resampled FWHMs of the emitting spot simulated as seen by the detector was considered, i.e. how well the emitting spot can be estimated under the assumption of the conditions in Table 3.2 based only on stochastic limitations (neglecting any potential systematic uncertainty). As mentioned earlier, for the assumed finite measurement time of 5 h the stochastic contribution to the error was most dominant. Figure 3.12 shows the fit of the logistic function as well as three selected resampled ESFs of the 1000 resampled ESFs for one geometry.

**Detector to Source Distance**

There is a tradeoff between the number of counts in the detector and geometric blur for the distance between the detector and the neutron emitting spot. If the distance is small, the count rate in the detector is higher due to the larger solid angle covered by the
Chapter 3. Development of Source Characterization Techniques

Simulate 100 edge positions, $x$, with MCNP6

Estimate number of counts, $I$, in detector

Fit ESF

Simulate new measurement by resampling from fitted ESF

Assume Poisson distributed number of counts

Fit ESF to resampled data

Compute FWHM

Obtain standard deviation of the distribution of 1000 FWHMs

Repeat 1000 times

Figure 3.11: Flowchart of the sensitivity study of the attenuating edge measurement

The ESF obtained from the MCNP6 simulation was resampled to investigate the sensitivity of geometric parameters for the experiment.
detector. However, to reduce geometric blur, one would either place the detector very close to the attenuating edge compared to the distance between source and attenuating edge, or put the detector very far away compared to the emitting spot diameter. The distance between the attenuating edge and the emitting spot was chosen to be as small as possible to enhance sensitivity to a small emitting spot and have minimal travel distance of the attenuating edge perpendicular to the path of neutrons from the source to the detector. Figure 3.13 presents the results for two selected source diameters. The spread in the estimated source FWHM is lowest for distances around 50 to 60 cm.

![Figure 3.13: Uncertainty of the FWHM as function of the detector distance](image)

(a) 2 mm source diameter.  
(b) 3 mm source diameter.

The final distance between detector and source was chosen to be 61 cm for mechanical reasons when assembling the structure that held the emitting spot size measurement.

**Attenuating Edge Thickness**

For a thicker attenuating edge the difference between the number of counts in the detector when the edge is completely covering the neutron source and when the path between source and detector is completely free of the edge is larger. However, a misalignment between detector, source, and attenuating edge in the case of a thicker edge blurs the source seen in the detector more compared to a thinner edge. This type of misalignment was not investigated in this work, assuming precise placement of detector and attenuating edge relative to the neutron beam path. Figure 3.14 indicates that the thicker the tungsten edge the smaller the spread in the estimated source FWHMs, given the ideal alignment between source, edge, and detector. The Figure shows only the results for the selected distance between detector and source. However, for the other investigated distances and source diameters, the trend was the same.
The final tungsten attenuating edge thickness was chosen to 2 cm because larger tungsten thicknesses provided only diminishing returns for a reduction in the spread of the estimated source FWHM. At the same time precise machining of a thinner high density tungsten slice was easier compared to a thicker one.

### 3.2.1.2 Experiment

The layout of the emitting spot size experiment is shown in Figure 3.15 including distances and dimensions of the tungsten attenuating edge, thickness of lead and copper shielding, as well as plastic scintillator. The $6 \times 6 \times 2$ cm$^3$ tungsten edge was aligned with the plastic scintillator using a laser that was fixed at the far end of the room. This laser was calibrated so that it pointed from the forward direction through the ion source aperture when the target was removed, i.e. along the $x$ axis seen in Figure 3.3 in $-x$ direction. The position of the attenuating edge close to the vacuum chamber of the neutron generator and the pink laser light can be seen in Figure 3.16. The edge was mounted on a linear motorized translation stage (MT1-Z812B) manufactured by ThorLabs, USA, that allowed remote control of the edge position.

The $5 \times 5 \times 20$ mm$^3$ PVT-based BC400 plastic scintillator supplied by St. Gobain [111], France, wrapped with aluminized mylar [63] was mounted in a custom-made 3D printed holder. An SiPM (ASD-RGB3S-P type supplied by AdvanSiD, Italy) with an active area of $3 \times 3$ mm$^2$ on a small printed circuit board was mounted against the back of the scintillator and connected to an Arduino Due-based readout system as detailed in Adams et al. [61]. The scintillator and the SiPM were placed inside a light tight, grounded copper box and connected via an RF feedthrough to the readout electronic board. To limit electromagnetic interferences known to occur when the RF ion source
was in operation, the readout electronics board and the Arduino Due were also placed inside a grounded copper Faraday cage. A lead shield was built up around the detector to limit unwanted detection of X-rays originating from electrons backstreaming from the target to the grounded ion source.

![Setup of the emitting spot size measurement](image)

**Figure 3.15: Setup of the emitting spot size measurement**
Distance between source and detector, detector sizes, lead, and copper thicknesses not to scale. Figure adapted from Kromer et al. [104].

![Photograph of the alignment of the tungsten edge](image)

**Figure 3.16: Photograph of the alignment of the tungsten edge**
The laser was aligned using the ion source aperture.

During the experiment, the detector response was recorded at 60 attenuating edge positions that were arranged in a random order to prevent any drifts in the behaviour of
the neutron source over time to influence the results. The edge positions were locally equally spaced, but closer to one another in the center of the ESF. At each edge position, the counts in the detector were integrated over around 300 s in 30 s readout intervals. This experiment was repeated three times, with a high voltage bias of the target of the neutron generator of around $\sim 75$ to $\sim 80$ kV, an averaged deuterium ion beam current between 1.0 and 1.3 mA read by the high voltage power supply, and a duty factor of the pulsed extraction electrode between 50 and 63%.

Before and after each experiment the number of counts without the neutron generator operating was recorded for one hour to allow for background correction. The background counts per time interval were taken as the mean between the two computed values $\frac{I_{BG}}{\Delta t_{BG}}$ with $\Delta t_{BG}$ being the duration of each background measurement. For each edge position the total number of counts $I_{meas}$ per measurement time $\Delta t_{meas}$ was corrected using the background measurement to yield the corrected count rate $C$:

$$C = \frac{I_{meas}}{\Delta t_{meas}} - \frac{I_{BG}}{\Delta t_{BG}}$$  \hspace{1cm} (3.8)

The total number of counts per time interval, $C$ was normalized by the average ambient dose rate, $H_{avg}$, read by an LB6411 neutron probe during the measurement interval at that edge position: $H_{avg} = \frac{\int_{t_1}^{t_2} H(t)\,dt}{t_2-t_1}$, where $\Delta t_{meas} = t_2 - t_1$. Hence the background corrected, dose normalized count rate, $\tilde{C}$, at each edge position reads:

$$\tilde{C} = \left( \frac{I_{meas}}{\Delta t_{meas}} - \frac{I_{BG}}{\Delta t_{BG}} \right) \frac{\Delta t_{meas}}{\int_{t_{meas}} H(t)\,dt}$$  \hspace{1cm} (3.9)

The experiment was repeated on three separate days and the recorded ESF with the fit of the logistic function from Equation 3.2 are plotted in Figure 3.17. The values computed from Equation 3.9 are normalized using the mean of the ESF when the attenuating edge is fully covering the path between detector and source. The edge position was centered for each experiment by taking the mean of edge fully withdrawn and fully inserted in the path between detector and source. The center position of the attenuating edge is then found by fitting a linear curve to the measurement points around the estimated symmetry position and taking the intersection between the mean of the prior estimated maximum and minimum values. The logistic fit was repeated 1000 times where for each fit the initial conditions to the optimizer using the Nelder Mead Simplex algorithm were sampled from a normal distribution [112]. The loss function of the optimizer was set as the total sum of squared differences between data points predicted from the logistic fit.
and the data points from the experiment. The mean of the FWHM labelled as “FWHM seen by the detector” for each measurement is summarized in Table 3.3 with an error that corresponds to the standard deviation of each respective set of FWHMs obtained from the 1000 fits.

Experiment number one resulted in a different FWHM and significantly higher uncertainty compared to the other two experiments. This is because during this experiment, especially during the four measurements at the edge positions when the edge was fully blocking the path between detector and source, there were more frequent high voltage sparks that influenced both the detector and the ambient dose rate reading in the LB6411 neutron probe. Experiments number two and three were recorded in the days following after experiment number one. The stability of the neutron generator in terms of high voltage breakdowns typically correlated with operating time after the vacuum system had been vented which was the case prior to experiment number one.

The experimental setup was modelled in MCNP6 as shown in Figure 3.15 and post-processed in the same fashion as described in Section 3.2.1.1. There were some minor differences in the MCNP6 models due to differences in the experimental setup that could not be foreseen when the experimental parameters were optimized. Firstly, as outlined earlier the Faraday cage was modified, allowing closer placement of the attenuating edge
to the source. The distance between source and attenuating edge front face was 55.5 mm. Secondly, two source definitions were modelled separately with MCNP6. The first source was modelled as a Gaussian distribution with FWHMs between 0.05 and 5 mm and the second was modelled from a uniform emission profile with radii between 0.2 and 4 mm. Figure 3.18 shows the ESF and computed Gaussian shaped source sizes for selected source FWHMs set in MCNP6 for this geometry.

![Fit of the logistic function to the ESF.](image)

(a) Fit of the logistic function to the ESF.  

![Computed LSF.](image)

(b) Computed LSF.

Figure 3.18: MCNP6 simulated ESF and corresponding Gaussian shaped spot size

Only a selection of source FWHMs in MCNP6 is shown. Figure adapted from Kromer et al. [104].

From these simulations, a lookup table was constructed that relates the FWHM seen in the detector to the FWHM that was set in the MCNP6 source definition for both Gaussian shaped source and uniform source definition. This lookup table is visualized in Figure 3.19. From this lookup table the emitting spot size FWHM was estimated to around 3 to 4 mm, as seen in Table 3.3 individually for each measurement. This value was larger compared to prior investigations done with this neutron generator in Zboray et al. [59] and Adams et al. [60] that estimated the emitting spot size in the order of 2 mm for a static target rod with a diameter of 12.7 mm. The neutron generator used for the experiments in this work used a rotating rod as the beam target, as shown in Figure 2.20. The pneumatic motor driving the rod with a V-belt drive exerted force on one end of the around 1 m long rod, creating a wobble on the opposite end of the rod close to where the ion beam was hitting the target. This lead to an overestimation of the physical neutron emitting spot size as on average the beam spot seen by the detector would be blurred slightly according to this motion. In other words, the effective neutron emitting spot for imaging purposes with the rotating target is slightly larger than the actual emitting spot on the target, because the target itself is moving slightly. For a fixed target configuration, the loading profile might only reflect the Gaussian distribution of the ion density in the beam, but as the neutron yield results from a product of the local
deuterium density in the target and local beam flux, the neutron production will be more flat than a Gaussian function. That renders the assumption about a negligible lateral diffusion of deuterium in the target questionable. A deeper analysis of this phenomenon was beyond the scope of this work.

![Emission profile](image)

**Figure 3.19: Lookup table relating the FWHM measured in the detector to the source FWHM**

Figure adapted from Kromer et al. [104].

<table>
<thead>
<tr>
<th>Experiment number</th>
<th>FWHM seen by the detector [mm]</th>
<th>Emitting spot FWHM (Gaussian) [mm]</th>
<th>Emitting spot FWHM (top-hat) [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.7 ± 0.2</td>
<td>3.3 ± 0.4</td>
<td>4.4 ± 0.2</td>
</tr>
<tr>
<td>2</td>
<td>2.3 ± 0.1</td>
<td>2.7 ± 0.1</td>
<td>3.8 ± 0.1</td>
</tr>
<tr>
<td>3</td>
<td>2.5 ± 0.1</td>
<td>3.0 ± 0.1</td>
<td>4.1 ± 0.1</td>
</tr>
</tbody>
</table>

**Table 3.3: Emitting spot FWHM of the Gen. I neutron generator**

The emitting spot was determined by fitting a logistic function to the recorded ESF and the emitting spot FWHM was estimated using the lookup table created with MCNP6.

The results overall indicate both stochastic uncertainty and a sensitivity to what emitting spot profile is assumed, in addition to potential systematic uncertainties which are assumed to be low but can only cause overestimation of the spot (i.e. conservative) as previously discussed. With better knowledge of the emitting spot profile, the emitting spot can therefore be better estimated, and this issue is revisited in later Sections after considering ion beam simulation results.
3.2.2 Ion Beam Simulations

The AC/DC \cite{113} and Particle Tracing Modules \cite{114} of COMSOL Multiphysics were used to model the electrical potential field and ion beam trajectories on the EULER cluster of the Swiss Federal Institute of Technology. COMSOL used the Maxwell equations with user defined boundary conditions and non-relativistic assumptions to compute the electric potential field. The boundary conditions in the simulation included the relative permittivity of materials, electric potentials at the material boundaries, ion beam release parameters, and conditions when the particles hit a wall of a defined material surface. For insulators, the zero charge boundary ensured that no displacement field could penetrate the boundary and discontinuity of the electric potential across the boundary. COMSOL divided the forces in the simulation into those due to external fields and interactions between particles. The external fields were computed from a finite element model. The electric potential field in this simulation was assumed stationary to significantly reduce computational cost by using a predefined bidirectionally coupled approach. In this iterative approach, COMSOL alternated between a stationary and time-dependent solver with user defined time stepping in the following way as detailed in the COMSOL User Guide \cite{114}:

1. Compute electric potential field using a stationary solver and provided boundary conditions. Set all contributions from particles to external fields to zero.

2. Compute all electric potential field variables using a stationary solver, using the contributions from particles to external fields computed in the previous step.

3. Compute the particle trajectories and their contributions to external electric potential field, using the field variables computed in the previous step.

4. Repeat steps 2 and 3 until the solution is converged after a predefined number of iterations has been reached.

The external electric potential field and the ion trajectories are directly coupled and the solution is significantly affected by the resolution of the mesh and time stepping in the above outlined iterative approach. In the model outlined later, space charge effects were significant in the extraction region near the ion source aperture and extraction electrode, because the ions had a low velocity magnitude and were in close proximity to each other. This influenced the electric potential field in this region which in turn influenced the shape of the beam significantly, in particular by enhancing the beam divergence or convergence. Both mesh and time resolution were investigated carefully and proved independence of the results on these parameters and overall validity of the solution.
3.2.2.1 Model

In the 3D model the target rod, vacuum chamber, copper aperture, extraction electrode, and turbomolecular pump were included as shown in Figure 3.20a. The components around the neutron source were not included because their position frequently changed and this would increase model complexity without significantly altering the electric potential field. The following boundary conditions were considered:

1. The target and extraction electrode surfaces were set to a defined negative potential. If not explicitly mentioned otherwise, simulations were set with a beam target negative high voltage of $-100\text{ kV}$ and an extraction electrode bias of $-3\text{ kV}$. The grounded surfaces of copper aperture (between ion source and accelerator column) and turbomolecular pump were modelled at ground potential. The borosilicate vacuum chamber was considered as an insulator. Figure 3.20b shows the resulting electric potential field in the simulation domain.

2. Surfaces of extraction electrode, vacuum chamber, and target were modelled with wall boundary conditions where the particle would stop if it hit a node at the wall.

3. Air with a relative permittivity of 1.0 was chosen in all model domains except in the walls of the vacuum chamber where a relative permittivity of 4.7 was taken [115].

4. The Infinite Element Domain was restricted to an inner radius of 1 m and a layer thickness of 0.1 m was considered in order to save computational cost. In this setting COMSOL stretches the coordinate system in that domain so that for all practical purposes, this domain is infinitely large. That means that the solution from a model with Infinite Element Domains will be the same as when the domain radius is increased. While this increases solution time and computational requirements, it removes the need to choose external boundary conditions or be concerned with the domain size. Both size of the domain and layer thickness were chosen as small as possible with insignificant influence on the magnitude of the electric potential field along the line at $y = z = 0$ in $x$ direction, where the $x$ direction denotes the direction in which the ion beam travelled (refer to Figure 3.20a for the coordinate system).

5. The ion beam current was assumed to be 1 mA. Each of the modelled particles represented a number of real particles per unit time. All particles of such a cluster move along the same path. This is a predefined option in COMSOL, making release of particles only during the first time step necessary and greatly reducing computational cost.
6. The plasma in the ion source was not modelled and the extracted ion beam current was assumed space-charged limited, in which case the Child-Langmuir law applies to the extractable current density [116]. Because of this and the small diameter of the extraction aperture, the plasma meniscus was assumed to be flat. The ion beam originated from this flat plasma boundary and ions were assumed to have full mobility.

7. Usually in a plasma generated with this type of system the electron temperatures are Maxwellian distributed in the range of 1 to 10 eV and the ions in most plasmas have a lower temperature in the order of less than 1 eV due to ineffective momentum transfer between electrons and ions [117]. In the ion beam simulations in this work, ions started with an initial kinetic energy of 0.15 eV and with a velocity vector perpendicular to the emitting surface. The spatial ion distribution on the beam target surface differed insignificantly when the initial kinetic energy was varied from 0.05 eV to 10 eV.

8. All ions were considered mono-atomic with charge state +1. For an ion source similar to the one used in this work Wu [87] found a ratio between impurities and atomic hydrogen ions of less than 10%.

9. The termination criterion for the iterative bidirectionally coupled solver outlined above was five fixed number of iterations. The solutions were usually steady after around three to four iterations.

(a) COMSOL model layout where the beam traverses in x direction. (b) Electric potential field in kV in the x-z plane. The outermost layer is the Infinite Element Domain.

Figure 3.20: COMSOL Multiphysics model to simulate the ion spot size on the target
Target high voltage −100 kV. Figure adapted from Kromer et al. [104].
3.2.2.2 Mesh Refinement

The custom-built mesh was refined on the material boundaries as well as inside the accelerator column, which is the space between the ion source aperture and the target. Several boundary layers were used in the extraction region. The total number of emitted particles was set to 3000 particles and the time stepping used in the time dependent solver was set to $2 \times 10^{-10}$ s. Variations of these two variables were found to have insignificant impact on the results. Models with four different meshes, summarized in Table 3.4, were created, where each model consisted of the same type of tetrahedral mesh elements, but with a different number of total mesh elements, which was controlled by setting the minimum size of the mesh elements in a domain in COMSOL. In each simulation, the charged particle distributions at different $x$ positions along the particle trajectories, i.e. different solution times, were evaluated. Figure 3.21 illustrates this analysis.

<table>
<thead>
<tr>
<th>Mesh identifier</th>
<th>Mesh elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>A (coarse)</td>
<td>670 000</td>
</tr>
<tr>
<td>B (normal)</td>
<td>830 000</td>
</tr>
<tr>
<td>C (fine)</td>
<td>3 800 000</td>
</tr>
<tr>
<td>D (finest)</td>
<td>5 500 000</td>
</tr>
</tbody>
</table>

Table 3.4: Number of mesh elements for the ion beam spot size simulation

For each time step ($x$ position) the distance between the trajectory and the centerline along which $y = z = 0$ held was computed for each of the 3000 trajectories. From all these measurements, an empirical cumulative distribution function (CDF) was constructed, which assigns each sample point a probability of $1/3000$. That means an increase of $1/3000$ in the empirical CDF at each sample point [118]. The empirical CDFs of the distances between the trajectories and the centerline for the different meshes were compared with the distribution using the finest mesh (D). To prove convergence of the solutions, the maximum absolute distances between any of the empirical CDFs using mesh A, B, and C with respect to the ones obtained with mesh D were computed [119]. The empirical CDF from mesh D was assumed to be the “true” distribution. Figure 3.22 shows this comparison of the empirical CDFs for one selected mesh, A, for one time step in the solution and Figure 3.23 shows the evolution of the maximum absolute differences for either of the three meshes with respect to the finest mesh D along the $x$ coordinate (different solution times). Mesh C was chosen as the final mesh.
Figure 3.21: Sketch illustrating the deuteron trajectory simulations
At various $x$ positions along the charged particle trajectory the distribution of the particle tracks was evaluated in the mesh refinement study. The whole beam trajectory inside the wireframe vacuum chamber is colored in red, hitting on the gray target surface. The zoomed out image in the $y-z$ plane shows a selected few of the charged particle tracks at one $x$ location, where the green dot is the centerline along $x$ (where $y = z = 0$). The two black arrows denote two distances of two example charged particle trajectories from this centerline. The overall upward shift, caused by the curvature of the electric field lines is addressed further in Section 3.2.2.3.

Figure 3.22: Illustration of the method to find the maximum difference in the distributions of the particle trajectories
The maximum difference between the empirical CDFs of the particle trajectories at one solution time step between mesh the coarse mesh, A, and the finest mesh, D, is shown.
3.2.2.3 Results

Results of the ion beam simulation for a target high voltage of $-100\,\text{kV}$, which is a typical operating value of the neutron generator, are shown in Figure 3.24. Due to the curvature of the electric potential field created by the grounded turbomolecular pump the simulated charged particles experienced a net force in the upward ($+z$) direction. As a consequence the ion distribution on the target surface is likewise shifted in $+z$ direction.

The (spatial) probability density function (PDF) of the ions on the target was estimated using a Gaussian kernel density estimator (KDE) that was included in the Python 3.7 package SciPy [112]. Results shown in Figure 3.25 were obtained for a high voltage setting of $-80\,\text{kV}$. This corresponds to the high voltage setting that the neutron generator was operating at when the emitting spot size experiment was carried out. A larger accelerating high voltage can lead to a focussing effect of the electric field and hence a smaller spot size on the target. From the estimated PDF the assumption of a Gaussian shaped emitting spot was verified. The FWHM of the emitting spot was estimated by taking a slice through center of the spot parallel to the $z$ and $y$ axis each and fitting a Gaussian function on the estimated PDF (Figure 3.25b). The emitting spot is shifted
Chapter 3. Development of Source Characterization Techniques

Figure 3.24: Ion particle trajectories and average kinetic energy

COMSOL simulation of the ion particle trajectories for a target accelerating voltage of $-100\,\text{kV}$. Figure adapted from Kromer et al. [104].

(a) Ion particle trajectories colored by average kinetic energy and electric potential field lines (red) in the $x$-$z$ plane. Note that the density of electric field lines is not proportional to the electric field strength.

(b) Ion particle trajectories in red and target surface colored in gray.

around 0.5 mm in $+z$ direction and larger in $z$ direction as compared to the $y$ direction. The trajectories extend around 3 mm in $y$ direction and around 3.8 mm in $z$ direction. This deformation comes from the shape of the target, which was a long rod that extended into the $z$ direction (see Figure 3.24b). Hence the electric potential field lines are curved around the target rod and focus the ion beam onto the target in the $y$ direction. On top of that the target being a rod had a curvature that was small compared to the spot, but deformed the spot in a 2D plot when the particle positions are mapped from the curved surface in 2D.

The FWHM of the ion beam spot on the target surface simulated in COMSOL is to some degree comparable to the FWHMs determined with the attenuating edge measurement setup assuming a Gaussian emitting spot, or diameters assuming a uniform disc (see Table 3.3). The distribution indicated by the simulations is a non-standard shape which appears somewhere between a uniform disc and a Gaussian profile. Therefore, for purposes of experimental spot size measurement, aside from stochastic uncertainty the reality is likely somewhere between the two look-up table options (Gaussian or uniform disc assumption). This assumes, however, as mentioned earlier that the distributions of ions on the target surface matches the distribution of neutron generation in the target. This might not be the case because of potential inhomogeneity of the loading with deuterium, which might distort the neutron emitting spot profile compared to the ion beam profile. In addition, further difference between simulation and experiment can originate
Chapter 3. Development of Source Characterization Techniques

Figure 3.25: Estimated spatial ion distribution on the target

The spatial ion distribution on the target was estimated using a Gaussian kernel density estimator. A Gaussian function is fitted on the PDFs along $y$ and $z$ direction each. The FWHM of the fitted Gaussian function is taken as the ion beam spot FWHM. Figure adapted from Kromer et al. [104].

from a small curvature of the target and, more importantly according to visual observation of the rod, a wobble of the target rod induced by the force of the V-belt that was driving the rotation of the target rod. Despite that, the effective emitting spot as seen by the detector is still likely to fall somewhere between the disc and Gaussian profile, meaning that the two look-up table options are likely still valid as a rough range in terms of determining the effective emitting spot. This wobble effect, however, can cause significant deviation between the simulated ion beam shape and the measured emitting spot, as was seen, with a difference of roughly 1 to 2 mm between the two.
Chapter 4

Generation II Compact D-D Neutron Generator at PSI

Several upgrades to the Gen. I compact D-D fast neutron generator at PSI were considered with the primary goal of increasing the neutron output while keeping the neutron emitting spot size small. Suppression of parasitic X-ray radiation was a secondary goal. The choice of upgrades, the considerations in their design, their installation, and an assessment of the performance of the upgrades are laid out in this Chapter. The new system is termed “Generation II” (or short “Gen. II”).

A new vacuum system with a different vacuum chamber, insulator, and copper aperture compared to the Gen I. design of the neutron source was designed. The extraction electrode assembly was modified to accommodate the same extraction electrode inside the copper aperture that was used previously in the neutron generator. To operate at lower deuterium gas pressures at high mono-atomic ion fraction and high power efficiency, a microwave ion source was adapted from an existing design. The last upgrade presented is an electric field method electron suppression electrode. Its intent was to limit backstreaming secondary electrons which produce Bremsstrahlung X-ray radiation when they are accelerated from the ion beam target at negative potential towards the grounded ion source.

4.1 Design of the Vacuum System

The main consideration that motivated a redesign of the vacuum system of the compact D-D fast neutron generator was the aim to improve the vacuum conditions inside the vacuum system to reduce high voltage breakdowns. The vacuum chamber of the
neutron generator can be simplified as a long, cylindrical pipe in a first order approximation. The conductance of piping in a vacuum system, expressed usually in m$^3$s$^{-1}$, is proportional to the diameter of the pipe in the case of such a long, cylindrical pipe [120]. The smaller diameter of the vacuum chamber of the Gen. I neutron generator design compared to the inlet of the turbomolecular pump used within the vacuum system (illustrated in Figure 2.1) required a conical reduction pipe that further limited conductance in the Gen. I design. A lower residual gas pressure inside the vacuum chamber, most importantly in the accelerator column — which is the space between beam target and ion source aperture — would result in a lower ionization rate of neutral gas particles, thus limiting backstreaming electrons which produce unwanted Bremsstrahlung X-ray radiation (see Section 4.3 for further details). On top that, a lower residual gas pressure reduces the probability of high voltage breakdowns that were limiting the stable operating high voltage of the neutron generator. As outlined earlier, a higher accelerating voltage (and hence higher deuteron energy) means a higher D-D reaction cross section (see Figure 1.2) which in turn increases the neutron output if all other parameters in Equation 1.8 are kept constant.

Practical considerations also motivated an adjustment of the Gen. I vacuum chamber. The planned installation of an electron suppression electrode in the Gen. I design was impractical due to the small space of 1 cm between the target and the inner wall of the borosilicate vacuum chamber (see Figure 2.15). On top of that, the planned implementation of a microwave ion source (for reasons outlined later) required a redesign of the copper aperture between the ion source and vacuum chamber. Figure 4.1 sketches the layout of the Gen. II neutron generator system. The distance between the bottom cap of the target rod and the surface of the turbomolecular pump was set so that the maximum electric field strength remained below the breakdown limit in vacuum. This influenced the length of the borosilicate insulator atop the vacuum chamber because the total length of the rotating target rod, developed in Chapter 2, was fixed. The dimensions of the corona rings that shielded the high voltage terminal from the ground potential to prevent high voltage breakdowns were chosen so that the maximum electric field strength remained below the breakdown limit in dry air. The distance between ion source aperture and target was adjusted to achieve a small ion spot size on the target — thus also achieving a small neutron emitting spot.

4.1.1 Vacuum Chamber Design

The inner diameter of the vacuum chamber was set to the diameter of the inlet of the turbomolecular pump (TM 520 supplied by Pfeiffer Vacuum AG, Switzerland), which is of type DN150. Stainless steel (304L) was chosen as the vacuum chamber material with
2 mm wall thickness. The total length of the vacuum chamber is 310 mm and was chosen so that the microwave ion source could be connected directly to the vacuum chamber. The vacuum chamber was produced by Kurt J. Lesker Company, United Kingdom.

Charged particle tracing and electrostatics simulations were set up in COMSOL Multiphysics to investigate the effect of the distance between ion source aperture and target surface (see Figure 4.1). The model, outlined in Figure 4.2, included the ion source aperture according to the design of the microwave ion source described in Section 4.2. Boundary conditions in the simulation were the same as in the descriptions outlined in Section 3.2.2.1 and the mesh was defined in the same way as the one used in the prior investigation of the emitting spot size (see details in Section 3.2.2.2).

The result of one simulation is shown in Figure 4.3. This simulation is representative for any of the simulations and results of the ion spot distribution in this Chapter, i.e. the shape of the beam spot was similar, but the size in \(y\) and \(z\) direction changed. Boundary conditions were considered as the ones described in Section 3.2.2.1. The estimated ion distribution on the target surface of the Gen. II neutron generator was more top-hat shaped than Gaussian (see Figure 4.3), contrary to what was the case in the simulation of the beam spot of the Gen. I neutron generator. Hence, a top-hat function was fitted to the ion distribution spot as highlighted in Figure 4.3. The extend of this top-hat fit
Figure 4.2: Layout of the electrostatics and charged particle tracing simulations in the design of the new vacuum system

The ion source region was modelled according to the newly adopted microwave ion source outlined in Section 4.2.

was used in this Chapter to assess effects on the neutron emitting spot size, keeping in mind however, that the ion distribution does not necessarily have to reflect the emitting spot size, as was discussed in detail when the technique was developed in Section 3.2.2.3.

Figure 4.3: Estimated spatial ion distribution on the target of the Gen. II neutron generator

The methodology for the simulations was the same as outlined in Section 3.2.2.

Results in Figure 4.4 showed that the higher the accelerating potential, the smaller the ion beam spot on the target in terms of fitted top-hat extend along either $y$ or $z$ axis. For reference on the coordinate system, see e.g. Figure 4.1. In the simulations, the extraction electrode was biased to $-3\text{kV}$ at a distance of 10 mm from the ion source.
front face. The decrease in spot size with increase in accelerating potential was larger along the $z$ direction compared to the $y$ direction. This was a result of the shape of the beam target as a long rod that shapes the electric potential field lines differently in the $z$ compared to the $y$ direction. From these results a small distance between ion source aperture and target is desirable. Practical considerations limited this distance to 88 mm. The diameter of the opening in the vacuum chamber is 80 mm, which is the same as with the Gen. I neutron generator design. That allowed re-use of the extraction electrode system that was used in the Gen. I neutron generator system with borosilicate vacuum chamber and RF-driven ion source.

![Figure 4.4: Effect of distance between ion source aperture and target as well as high voltage on estimated ion spot size](image)

The charged particle tracing simulations showed that a small distance between ion source aperture and target surface results in a small ion beam spot size on the target.

A design constraint for the distance between the bottom cap of the target and the upper boundary of the turbomolecular pump was that the maximum electric field strength on the target surface must remain below $8 \text{kV mm}^{-1}$ to prevent high voltage breakdowns [121]. Electrostatics simulations with COMSOL Multiphysics were carried out and the maximum electric field strength was recorded, as displayed in Figure 4.5. Figure 4.6 shows the maximum electric field strength for various distances between the bottom cap and the turbomolecular pump.

The maximum electric field strength remained below the limit of $8 \text{kV mm}^{-1}$ for distances between the target bottom cap and turbomolecular pump surface larger than
around 30 mm. On top of this analysis, great care was taken to ensure the smoothness and cleanliness of surfaces inside the vacuum system. As outlined by Descoeudres et al. [122], the high voltage breakdown mechanisms in vacuum differ from the ones in air. The emission of electrons from the cathode by field emission originating from so-called micro-protrusions were considered to play a major role in voltage breakdowns between metallic electrodes in a high vacuum. A smoother surface would thus have fewer micro protrusions that would reduce the breakdown probability.

### 4.1.2 Insulator Design

A 365 mm long, DIN150 borosilicate insulator supplied by Buchiglas, Switzerland, provided electrical insulation between the grounded vacuum chamber and the high voltage terminal on top of the insulator (see Figure 4.1). Two shielding corona rings were placed at high voltage and ground potential each. The dimensions of the rings were considered to reduce the maximum electric field strength and the total length of the insulator was chosen so that the maximum electric field strength between the two shielding corona rings was below the breakdown voltage of 3 kV mm$^{-1}$ [123] (dry, ambient air at 1 bar) for a target high voltage setting of $-150$ kV. This value, $-150$ kV, was taken as the design value because it was the maximum high voltage that could be supplied by the currently used high voltage power supply that was the same as with the Gen. I neutron generator (SR-150-N-300 from Technix, France). A 2D axis-symmetric electrostatics simulation with COMSOL Multiphysics showed that the maximum electric field strength on the surfaces was 1.3 kV mm$^{-1}$ for the chosen dimensions of the corona rings and length of insulator. Figure 4.7 shows the electric potential field resulting from the 2D study.
Boundary conditions in the simulation were similar to the descriptions outlined in Section 3.2.2.1. The electrostatics simulation with COMSOL Multiphysics was set up as a 2D axis-symmetric simulation with the symmetry line at $r = 0$ going through the target rod. Structures shaded in red in the Figure were biased at the negative potential. The maximum electric field strength on the corona ring surfaces in the final design remained well below the nominal breakdown field strength of air.

The two hand-polished corona rings were made of stainless steel (304L) and were assembled from eight pipe bends supplied by Kohler AG, Switzerland, welded into two rings. The pipe bends had a bend radius of 205 mm, a pipe diameter of 88.9 mm, and a wall thickness of 2 mm. Two custom-made silver coated copper gaskets with an FKM (fluoroelastomer) O-ring each pressed to the outside of the gaskets were used on the sealing surfaces of the borosilicate insulator and pressed with a DN150 flange ring each provided by Buchiglas, Switzerland, to the respective opposite, custom-made sealing surfaces.

### 4.1.3 Copper Aperture Design

The copper aperture with an outer diameter of 175 mm and a thickness of 15 mm which connected the vacuum chamber and the microwave ion source was designed in three different parts. It was water-cooled to protect the FKM O-rings on either side of the
Chapter 4. *Generation II Compact D-D Neutron Generator at PSI*

Figure 4.7: Electrostatics potential field simulation outside the vacuum chamber

The 2D electric potential field simulation was used to design the insulator and corona rings. Components shaded in red were biased to high negative potential. Electric potential field lines are not proportional to the electric field strength.

aperture from failing, held the extraction electrode electrically insulated in place, and allowed feedthrough of the extraction electrode bias voltage of nominal $-3 \text{kV}$. The coolant lines were designed to be as close to the center of the aperture as possible to protect the FKM O-rings. An alumina tube was inserted below a DIN16 flange to provide electrical insulation between the grounded copper surfaces and the copper wire transmitting the extraction electrode voltage (nominal $-3 \text{kV}$). On the opposite side, a DIN16 flange was connected to allow mounting of a pressure gauge (PKR 251 compact full range pressure gauge supplied by Pfeiffer Vacuum AG, Switzerland) to monitor the pressure level in the extraction region and to accommodate a valve for faster evacuation of the deuterium gas supply line. The different parts of the copper aperture and connections to it (DIN16 flanges and steel pipes) were joined using vacuum brazing. The CAD (computer aided design) showing the final design of the whole copper aperture assembly is shown in Figure 4.8.

The extraction electrode was mounted between two plates of MACOR [124] insulators, manufactured by Goodfellow Cambridge Ltd., United Kingdom, with a small copper ring in between. The wire from the pulsed extraction voltage generator was connected to this copper ring. Zirconia screws and nuts were supplied by Ceramco Inc., USA, and used to fix the extraction electrode system (shown in Figure 4.8) together and connect it to the copper aperture. Figure 4.9 shows a photograph of the front side of the copper aperture with the extraction electrode mounted in place and Figure 4.10 shows the aperture from the opposite site when it was connected to the vacuum chamber.
Charged particle tracing simulations with COMSOL Multiphysics, referenced in Figures 4.2 and 4.3, were set up with the beam target rod biased to $-100\text{kV}$ and the ion beam current set to $0.2\text{mA}$. Figure 4.11 summarizes the results of these simulations, where the top-hat extend of the ion beam spot on the target was estimated for different extraction electrode voltages and offsets, i.e. the distance between the front face of the ion source and the back side of the extraction electrode. A larger offset decreased the spot size, other variables kept constant, which is desired for imaging applications due to a reduction in imaging blur as discussed in Section 1.1.2. However, from the perspective of ion beam extraction, a smaller offset is favorable, because this increases the
extractable current density. The offset was chosen to 10 mm limited by the zirconia nuts and screws that fixed the extraction electrode assembly (see Figure 4.10).

Figure 4.10: Photograph of the extraction holder and copper aperture from its back side mounted on the vacuum chamber

The extraction voltage was planned to be varied later in the experimental phase and compared to the simulation results. Unfortunately, overheating of the extraction electrode prevented this investigation, see details in the Appendix B.

Figure 4.11: Effect of extraction voltage and offset on ion spot distribution

(a) Spot size depending on the extraction bias voltage. Offset fixed to 10 mm. (b) Spot size depending on the offset of the extraction electrode. Extraction voltage fixed to −3 kV.

The larger the extraction voltage, the larger the estimated ion spot size on the target surface. The larger the distance between the extraction electrode and the ion source aperture (i.e. offset), the smaller the ion spot size. Results were obtained from charged particle tracing simulations with COMSOL Multiphysics.
4.2 ECR Microwave Ion Source Design

ECR (electron cyclotron resonance) microwave ion sources have a proven track record of stable high ion beam currents, high mono-atomic species fraction, high power efficiency, and can operate at low process gas pressures in the ion source cavity in the order of \(1 \times 10^{-3}\) mbar \([125, 126, 127, 128, 129, 130, 131]\). This makes such an ion source system a promising candidate to align with the previous outlined goals of reducing high voltage breakdowns inside the vacuum system of the neutron generator by reducing the residual gas pressure in the vacuum chamber.

4.2.1 Design Considerations

In the context of D-D or D-T neutron generators, ECR microwave ion sources have been developed for medium sized systems, such as Cockroft-Walton type sources \([132]\), but also compact sources \([127, 129]\). Ions are created in a resonator when the entering microwave power transmits energy to free electrons which, provided enough energy was transmitted to the electrons, ionize the neutral deuterium in the plasma chamber by colliding with neutral gas species. In an ECR type ion source, the frequency of the microwave radiation coincides with the angular frequency of rotation of the free electrons \([116]\). Without the ECR effect, the power required to ignite the plasma in a typical microwave ion source would be significantly higher \([133]\). The angular frequency of the electron motion is coupled to the magnetic field in which the electrons propagate. This magnetic field can be either created by means of solenoid coils (electromagnets) or with permanent magnets. The latter offer better reliability because no power is required to create the magnetic field and fewer parts need to be maintained \([134]\). For a microwave frequency of 2.45 GHz the magnetic field required to establish the electron resonance condition is 875 G \([116]\). In permanent magnet type ion sources, usually NdFeB or SmCo type magnets are used. The main differences to consider between the two types for use with the compact D-D fast neutron generator are thermal stability and resistance to radiation. SmCo is more temperature resistant towards demagnetisation compared to NdFeB and shows a higher radiation resistance, as investigated for example in Croat et al. \([135]\) or surveyed by Shepherd \([136]\). The effect of neutron irradiation on NdFeB magnets was assessed in Waldmann and Ludewigt \([128]\), who concluded that the NdFeB magnets would have to be replaced after 3200 h of D-D and after 100 h of D-T operation with neutron yields of around \(1 \times 10^{10} \text{s}^{-1}\) and around \(5 \times 10^{11} \text{s}^{-1}\), respectively. SmCo magnets, compared to NdFeB magnets, can withstand around six orders of magnitude higher neutron fluence before magnetic flux loss occurs \([137]\).
For D-D or D-T fast neutron generators, ECR microwave ion sources have for example been developed and characterized thoroughly in Waldmann and Ludewigt [127, 128] or by Ji [129]. Waldmann and Ludewigt [127] developed an ECR microwave ion source for a (sealed) compact high-yield neutron generator. The microwave, equipped with NdFeB permanent magnets, operated at 2.45 GHz with 400 W and was designed to produce a 100 mA ion beam current extracted through a $60 \times 6 \text{ mm}^2$ slit aperture. They found that the wall material of the ion source chamber played a significant role in increasing the ion beam current density and mono-atomic ion fraction. In Waldmann and Ludewigt [128] they documented that the proton fraction was highest with boron nitride layers on the front and back walls of the ion source compared to other wall materials. They also observed that the extracted ion beam current density increased with the microwave power (linearly in the range of 400 to 600 W) and increased with decreasing pressure inside the ion source, which was also observed with experiments in the ion source adopted in this work. Roychowdhury et al. [138] found as well that the ion chamber wall material had a significant impact on the mono-atomic ion fraction and confirmed the superiority of boron nitride over other wall materials. They attributed the enhanced mono-atomic ion fraction to the reduction of wall recombination processes and boron nitride having a high secondary electron emission coefficient. The former hinders the formation of molecular ions on the chamber wall surface and the latter enhances the electron density in the ion source which increases the ionization probability of the process gas. Both effects would net increase the production of protons.

### 4.2.2 Mechanical Design

The compact ECR microwave ion source used in this work has been developed for PSI’s high intensity proton accelerator and was essentially a copy of this system described and benchmarked in detail in Baumgarten et al. [130]. The source has shown high reliability in delivering an around 10 mA proton ion beam for over 2000 h continuous round the clock operation. The CAD design of the components for use and documentation in this work was provided by Dietmar Götz\(^1\) based on the developments described in Baumgarten et al. [130]. Figure 4.12 shows a CAD image of the whole assembly and Figure 4.13 is a photograph of the microwave line in this present work connected to the vacuum chamber of the upgraded neutron generator. Figures 4.14 and 4.15 depict the assembly connected to the vacuum chamber viewed as a horizontal and vertical cut, respectively.

A ferritic front plate (StW22, DD11 1.0332) with a tapered tungsten insert served as a magnetic mirror and as a shield towards the extraction region. In the original design of

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Figure 4.12: Overview of the components that made up the microwave ion source
Components indicated with a star were developed in Baumgarten et al. [130].

Figure 4.13: Photograph of the microwave ion source fully assembled
Components indicated with a star were developed in Baumgarten et al. [130].
Figure 4.14: Horizontal cut through the microwave waveguide
Components indicated with a star were developed in Baumgarten et al. [130].

Figure 4.15: Vertical cut through the microwave waveguide
Components indicated with a star were developed in Baumgarten et al. [130].
the microwave ion source, the aperture in the tungsten piece had a diameter of 5 mm. This was adjusted to 1 mm for the use in the compact D-D fast neutron generator system to decrease the neutron emitting spot size for the sake of an earlier outlined reduction of blur in fast neutron transmission imaging applications (see Section 1.1.2). Three rings of Sm$_2$Co$_{17}$ permanent magnets (VACOMAX 225 supplied by Vakuumschmelze, Germany) created the 875 G magnetic field ECR resonance at 2.45 GHz inside the ion source chamber. A magnetostatics COMSOL Multiphysics simulation is compared to measurements of the magnetic field configuration along the centerline of the magnet rings in Figure 4.16. Simulation and experiment were found in good agreement given the difficulty of fixing the measurement probe and hence its position in the strong magnetic field. Figure 4.17 is a photograph of the magnets assembled and connected to the vacuum chamber.

![Figure 4.16: Measurement and simulation of the magnetic field inside the microwave ion source](image)

The three rings of Sm$_2$Co$_{17}$ permanent magnets created an axial magnetic field that was simulated with COMSOL Multiphysics. The shaded blue region depicts the uncertainty in the positioning of the magnetic field probe.

The 50 mm diameter, 38.5 mm long vacuum chamber was made out of aluminum nitride with an aluminum oxide lid. A pressed copper gasket sealed the aluminum oxide and aluminum nitride parts of the ion source chamber. The length of the ion source chamber was optimized in Baumgarten et al. [130] to correspond to a quarter of a wavelength for a 2.45 GHz microwave in a WR284 waveguide and the radius corresponded to twice the maximal radial extension of ECR resonance zone. Flow of deuterium into the vacuum
The rings were connected to the vacuum chamber with the custom-made, water-cooled copper aperture. Components indicated with a star were developed in Baumgarten et al. \cite{130}.

The chamber was monitored and controlled using an elastomer sealed mass flow control meter (SLA5850 REV B) that was calibrated for hydrogen and supplied by BROOKS Instrument GmbH, Germany.

Two water-cooled copper plates were used to remove heat from the permanent magnets and prevent demagnetization. Two high temperature resistant O-rings (type KALREZ supplied by Ap soparts, Switzerland) were used as vacuum seal between the aluminum oxide lid and a custom-made water-cooled copper holder as well as between this holder and the ferritic front plate. A modified WR284 waveguide (supplied by Richardson Electronics GmbH, Germany) with a custom-made four step rectangular to ridged binomial matching transformer to match the plasma impedance and concentrate the microwave power into the centerline of the plasma chamber (along the $x$ axis) was slid into the water-cooled copper holder structure. The waveguide was modified to accommodate two air cooling lines on its side that blew cold air created with two vortex tubes (BP3908J supplied by Eputec GmbH, Germany) on the back side of the ion source chamber. Baumgarten et al. \cite{130} had investigated boron nitride as a chamber material in earlier iterations of the microwave ion source, but observed a low lifetime of the plasma chamber attributed to a combination of plasma etching of the chamber walls and high voltage breakdowns created by the deposition of boron nitride dust on the extraction electrodes. A coaxial to waveguide adapter, manufactured by Fricke und
Mallah GmbH, Germany, was flanged at the far end of the modified WR284 waveguide and connected to a 2.45 GHz, 200 W, air cooled solid state microwave generator (GMS200WSM56MPFCFME1IRVFAIT D supplied by SAIREM, France).

### 4.3 Electron Suppression Electrode Design

Backstreaming electrons can either be created by kinetic emission of secondary electrons under ion bombardment of the beam target [139] or by ionization of residual neutral gas particles in the accelerator column [131]. In the compact D-D fast neutron generator, backstreaming secondary electrons were accelerated in the high potential field and streamed away from the beam target (which was biased at high negative potential) towards the grounded ion source. The resulting electron beam struck and heated up the extraction electrode and lead to release of particles from the extraction electrode which increased risk of high voltage breakdowns. On top of that, while the electrons were slowing down, characteristic Bremsstrahlung X-ray radiation was produced that created unwanted signals for example in the scintillators used for fast neutron detection described by Adams [40]. Additionally, the secondary electrons formed a leakage current that superimposed on the ion beam current measured by the high voltage power supply making determination of the true ion beam current difficult.

To reduce the amount of the backstreaming electrons created by ionization of neutral gas particles in the accelerator column, the residual gas pressure level was lowered by improving the vacuum design of the upgraded neutron generator as outlined in Section 4.1 and adopting the ECR microwave ion source described in Section 4.2. Secondary electrons emitted from a titanium target surface under bombardment with 100 keV protons typically have kinetic energies of around 10 to 30 eV [139, 140]. Hasselkamp et al. [141] found that for 100 keV protons, around 1.5 electrons per incoming projectile were liberated from a titanium surface. Large and Whitlock [142] determined that the number of liberated electrons was the same for deuterons as for protons at the same energy and found that 1.2 electrons were liberated from a titanium surface per incoming 100 keV deuteron.

For compact D-D or D-T fast neutron generators the quantity of backstreaming electrons can be limited by means of magnetic or electric suppression. Suppression by a magnetic field relies on the deviation of the (negatively charged) electrons in the presence of the magnetic field. In electric field suppression, a so-called electron suppression electrode is enclosing the beam target with an aperture opening to let the ion beam pass through. By biasing the suppression electrode to a higher absolute negative potential compared to the target, secondary electrons emitted from the target are pushed back to the target by
the electric field between the target and the suppression electrode. Figure 4.18 outlines this electric field suppression principle for the neutron generator used in this work.

(a) No suppression electrode: Secondary electrons are released from the target surface under the bombardment with deuterium ions. The electrons stream back accelerated in the electric potential field between target and grounded ion source and release Bremsstrahlung X-ray radiation when slowing down.

(b) With suppression electrode: The suppression electrode is biased at a higher negative potential compared to the target and thus hinders secondary electrons emitted from the target surface from streaming back to the ion source.

Figure 4.18: Sketch of the electric field method to stop backstreaming secondary electrons

Wu [87] used seven Zener diodes in reverse bias connected to an electric suppression electrode around the beam target of an D-T neutron generator that operated at $-80$ kV. Waltz et al. [143] investigated both magnetic and electric suppression in an high flux D-D neutron generator. They found full electron suppression and a reduction of Bremsstrahlung X-ray radiation by a factor of around 20 using an electron suppression electrode that was biased at a higher negative potential compared to the target using a stack of reversely Zener diodes providing an 800 V drop between the target (at $-100$ kV) and the suppression shroud. They also investigated magnetic suppression with an 800 G magnetic field generated by neodymium magnets of grade N50 around the beam target, but found that the electrons were not as effectively suppressed as compared with the electric field suppression technique. Huang et al. [98] also investigated both magnetic and electric electron suppression for the design of their compact D-D neutron generator. From their simulations they concluded that magnetic suppression would be as effective as electric suppression, but the demagnetization of the permanent magnets as a result of heat conduction from the target made electric suppression more attractive. The voltage drop between the beam target and the electron suppression electrode was designed to be created by an 0.5 MΩ resistor. Huang et al. [144] later tested their earlier design
simulations in an experimental campaign and confirmed the effectiveness of the electric field suppression method at deuteron energies of 80 to 120 keV and ion beam currents between 1 and 4 mA. Magnetic field suppression was considered inferior compared to electric field suppression for the aforementioned reasons of demagnetization. After this review, the electric field suppression method was adopted in this work.

4.3.1 Electrostatics and Charged Particle Tracing Simulations

![Figure 4.19: Electrostatics simulations with COMSOL Multiphysics to dimension the electron suppression electrode](image)

Electrostatics and charged particle tracing simulations with COMSOL Multiphysics (see Figures 4.2 and 4.3) were taken into consideration to ensure that the maximum electric field strength in the vacuum chamber remained below the aforementioned critical value of 8 kV mm\(^{-1}\) and to investigate the effect of the suppression electrode design on the neutron emitting spot size. These simulations were performed for different suppression electrode aperture diameters and dimensions of the rings around the aperture and at the bottom end (in \(z\) direction) of the suppression electrode as outlined in Figure 4.19. The ion beam current was set to 1 mA and other boundary conditions were the same as outlined in Section 3.2.2.1. The mesh was set up following the same methodology described in Section 3.2.2.2.

The electric field suppression method was evaluated using the direction of the electric field vector in the \(x-y\) plane (at \(z = 0\)) for a target high voltage bias of \(-100\) kV, as shown in Figure 4.20. This method was adopted from Waltz et al. [143], where the criterion for
Figure 4.20: Distribution of the electric field strength in the deuteron beam plane

The electric field strength in $x$ direction near the target surface is negative, thus pushing the electrons back to the target. $x$-$y$ view cut through the plane at $z = 0$ mm. Green lines correspond to 0 kV mm$^{-1}$ electric field strength in $x$ direction.

Figure 4.21: Optimization of the shape of the electron suppression electrode

The electron suppression electrode was shaped so that the maximum electric field strength for $-100$ kV remained below 8 kV mm$^{-1}$ [121]. $y$-$z$ view cut through the target centerline.
effective electric field suppression was that the net electric field strength in \( x \) direction was negative in the region between the electron suppression electrode and the target. When the secondary electrons are liberated from the target, a net positive electric force in \( x \) direction will accelerate them towards the ion source. If on the other hand the electric field strength in \( x \) direction is negative near the target, secondary electrons are accelerated in the opposite direction, i.e. back onto the target. The maximum electric field strength on the surface of the extraction electrode at \(-100\) kV remained below the critical value of 8 kV mm\(^{-1}\) for the final suppression electrode design as shown in Figure 4.21. The maximum electric field strength occurred at the bottom of the suppression electrode and could be adjusted by moving the suppression electrode in axial (\( z \)) direction or modifying the curvature of the shielding ring at the bottom.

\[\text{Figure 4.22: Effect of the electron suppression electrode on backstreaming electrons}\]

Simulation with COMSOL Multiphysics of the effect of the electron suppression electrode on backstreaming electrons. Note the different scales in the two colorbars.

Figure 4.22 compares the trajectory of secondary electrons using a charged particle tracing simulation with COMSOL Multiphysics. For this simulation, the electron beam current was set to 0.6 mA, assuming 1.2 electrons per incident 0.5 mA deuterium ion beam. The electrons were released according to the probability density corresponding to the deuterium ion tracks that arrived on the target surface obtained from charged particle tracing simulations presented in Figure 4.19 for a deuterium ion beam current of 0.5 mA at a target high voltage of \(-100\) kV. The electrons were released in \(-x\) direction with an initial kinetic energy of 30 eV [139, 140]. Without the suppression electrode, secondary electrons were accelerated towards ion source or extraction electrode. Yet, with a suppression electrode biased to a higher negative potential of \(-100\) kV around
the beam target, secondary electrons were accelerated back towards the target, which was biased to $-98.6 \text{kV}$.

The influence of the bias voltage of the suppression electrode on the beam spot size, shown in Figure 4.23, was found to be negligible in charged particle tracing simulations with COMSOL Multiphysics for an extraction electrode voltage of $-3 \text{kV}$ and an ion beam current of $0.5 \text{ mA}$ for an accelerating potential of $-100 \text{kV}$. The spatial ion distribution on the surface was similar in shape to the one shown in Figure 4.3. A higher target high voltage bias was found to have a much stronger focusing effect on the spatial distribution of ions on the target surface, which agrees with results shown in Figure 4.4 where no suppression electrode was included in the simulation. The smaller top-hat extend for any one accelerating potential for the case with suppression electrode compared to without can be attributed to the smaller distance between the high voltage terminal and the grounded ion source. This was already observed in Figure 4.4 where a smaller distance produced a smaller ion beam spot size.

![Figure 4.23: Effect of bias voltage and overall accelerating potential on ion spot size](image)

(a) There is no significant influence of the high voltage bias of the suppression electrode on the ion spot size on the target surface. Accelerating potential was $-100 \text{kV}$.

(b) The higher the accelerating voltage, the smaller the ion beam spot size on the target. Suppression electrode bias was $-1.4 \text{kV}$. With the suppression electrode, the ion spot size is smaller compared to the case without the suppression electrode.

The final design of the suppression electrode, shown in Figure 4.24, had a suppression electrode aperture of $10 \text{ mm}$ and an inner diameter of $50 \text{ mm}$, i.e. the distance between the target surface and the inner surface of the suppression electrode was $5 \text{ mm}$. The wall thickness of the electron suppression electrode was $4 \text{ mm}$ everywhere except for the region near the suppression electrode aperture where the thickness was increased to around $10 \text{ mm}$ to make manufacturing easier. Edges of the suppression electrode
and especially the suppression electrode aperture were carefully rounded to reduce the electric field strength and avoid high voltage breakdowns.

### 4.3.2 Mechanical Design

Figure 4.24 shows the electron suppression electrode as a CAD model and a photograph after it was assembled. The stainless steel lid was placed on top of the borosilicate insulator and had a DIN16 flange for the voltage feedthrough to the suppression electrode that was made out of aluminum. The upper cylindrical parts of the suppression electrode with an internal diameter of 58 mm and a wall thickness of 4 mm were fixed with zirconia screws (manufactured by Ceramco Inc., USA) to the stainless steel lid, where three MACOR insulators (supplied by Goodfellow Cambridge Ltd., United Kingdom) provided electrical insulation between the stainless steel lid that was biased at the same potential as the beam target. The lower cylindrical parts of the suppression electrode (with 50 mm inner diameter) were designed to allow for sliding the aperture in the suppression electrode in the $z$ direction. In combination with free rotation of the stainless steel lid in the $x$-$y$ plane this allowed alignment of the aperture in the suppression electrode with the ion source aperture. The $z$ direction was fixed after assembling the suppression electrode using four silver screws that were designed for use in high vacuum conditions. To enable easy changing of the size of the aperture in the suppression electrode, its lower section was cut into three separate parts where the centerpiece was threaded at its end. If the ion source aperture diameter was to be changed, e.g. to allow for a higher extracted ion beam current density and consequently an increased neutron output (at the cost of an increase in neutron emitting spot size), the aperture in the suppression electrode could be easily exchanged without manufacturing the whole electrode from scratch.

![Figure 4.24: CAD model and photograph of the electron suppression electrode](image)
The voltage drop between the target and the suppression electrode was maintained using seven reversely biased ZX200 Zener diodes manufactured by DSI, Singapore, in series as sketched in Figure 4.25. The arrangement of Zener diodes was chosen following the developments in Wu [87] and in Waltz et al. [143]. Each of the seven diodes provided a voltage drop of 200 V, hence the whole assembly represented a voltage regulator, achieving the design voltage drop of 1400 V between target and suppression electrode. A set of eight high power 100 MΩ resistors (ROX300100MGNF5 supplied by Vishay Intertechnology Inc., USA) was connected in series between high voltage and ground to ensure a small current flowing through the circuit and hence that the Zener diodes provided their voltage regulating function.

![Diagram of the reversely biased Zener diodes](image)

**Figure 4.25: Diagram of the reversely biased Zener diodes**

Each of the seven diodes provided a voltage drop of 200 V, totalling a voltage drop of 1.4 kV between the beam target and the electron suppression electrode.

### 4.3.3 Validation

The voltage difference between beam target and electron suppression electrode was measured by connecting a 22 kΩ resistor in series between the 800 MΩ resistor stack and the ground. Figure 4.26 displays the corresponding curve between expected and measured beam target high voltage given the 1.4 kV voltage drop over the seven Zener diodes.
For high voltages between $-10$ to $-70\text{kV}$ the expected voltage agreed well with the measured voltage, yet beyond $-70\text{kV}$ the averaged current, read by the instrument of the high voltage power supply, increased significantly due to leakage currents making the measurement unreliable at higher voltages. The overall behaviour extrapolated from the lower voltages suggested that the Zener diode stack performed as designed and laid out in Wu [87] and Waltz et al. [143].

![Figure 4.26: Validation of the voltage drop between electron suppression electrode and beam target](image)

The current refers to the averaged target current measured by instrument of the high voltage power supply.

### 4.3.4 Leakage Current Measurement

With the electron suppression electrode and the Zener diode circuit connected as sketched in Figure 4.25 in the Gen. II neutron generator system, the averaged target current measured with the instrument of the high voltage power supply was significantly higher than the averaged target current measured in the Gen. I design.

During operation of the Gen. I neutron generator, the averaged target current read by the instrument of the high voltage power supply, $I_{\text{avg}}$, was comprised of the averaged leakage current, $I_{\text{leak}}$, the averaged current due to secondary backstreaming electrons, $I_e$, and the true averaged beam current due to the deuterium beam, $I_{\text{ion}}$ [144]:

$$I_{\text{avg}} = I_{\text{leak}} + I_e + I_{\text{ion}}$$
In the Gen. II design, the electron suppression electrode aimed to suppress secondary backstreaming electrons. Assuming perfect suppression \((I_e = 0)\), Equation 4.1 can be rearranged to find the true averaged ion beam current, \(I_{\text{ion}}\):

\[
I_{\text{ion}} = I_{\text{avg}} - (I_{\text{leak}} + I_e)
\]

\[
\approx I_{\text{avg}} - I_{\text{leak}}
\]  

The averaged leakage current, \(I_{\text{leak}}\), can be determined when the microwave generator is shut off, i.e. high voltage is supplied to the suppression electrode and beam target but no plasma is ignited in the microwave ion source. This does assume that there is no influence of the microwave radiation on the reading of the averaged target current. In the Gen. I design, the RF-field induced electromagnetic interference in nearby electronic devices but this was not observed with the microwave driven ion source in the Gen. II neutron generator.

![Figure 4.27: Averaged leakage current as a function of the high voltage power supply](image)

The averaged leakage current was read by the instrument of the high voltage power supply. The microwave generator was turned off and the voltage drop between target and electron suppression electrode was 1.4 kV.

Figure 4.27 shows the reading of \(I_{\text{leak}}\) using the instrument of the high voltage power supply. This curve served as an important indicator of the upper limit of operation of the neutron generator in terms of beam current with the present high voltage power supply,
that had a maximal high voltage rating of \(-150\) kV and maximum current rating of 2 mA. For example at \(-100\) kV, a leakage current of 0.2 mA limited the ion beam current to at most 1.8 mA assuming no current due to secondary backstreaming electrons. Using Figure 4.27 as calibration curve, the averaged ion beam current in the Gen. II design due to the deuterium beam, \(I_{\text{ion}}\), could be estimated using Equation 4.1.

### 4.4 Neutron Generator Performance

The final design of the Gen. II compact D-D fast neutron generator is summarized in Figure 4.28. The individual components, outlined in earlier Sections 4.1, 4.2, and 4.3 are split apart for visualization but were assembled together towards the direction of the respective port of the vacuum chamber. Figure 4.29 is a photograph of the system including most of the components visible with the exception of the cooling unit of the microwave power supply and the LB6411 Berthold neutron probe that was placed at \(y = 70\) cm and was covered by the vacuum chamber in the photograph.

A revised MCNP6 model for the Gen. II neutron generator was set up following the same methodology as for the Gen. I neutron generator outlined in detail in Section 3.1. This model took all the changes to the Gen. I neutron generator into account with
the same assumptions, i.e. omitting piping, cables, and components further away from the neutron source because they had negligible impact on the neutron flux. Using this model, the ambient dose rate read in the LB6411 neutron probe was used to estimate the total neutron output for the Gen. II neutron generator.

4.4.1 Operational Results

The extraction electrode failed during the initial testing phase of the Gen. II neutron generator due to poor heat removal from the MACOR insulator. Details are addressed in the Appendix B. Thus, the results shown in this Section refer to the Gen. II neutron generator system outlined in Figure 4.28 without the extraction electrode inside the copper aperture.
Figure 4.30 shows the loading of the fresh, deuterium-free target of the Gen. II neutron generator. The electron suppression electrode was biased 1.4 kV compared to the beam target and was set to a high potential of $-100$ kV, the microwave generator operated at a forward setpoint power of 200 W, at a reflected power of around 5 to 10 W, and at a microwave frequency of 2.44 to 2.45 GHz. The latter was automatically adjusted by the microwave generator unit. Unless otherwise specified, the microwave generator operated at these conditions during typical operation. There were a few high voltage breakdowns that gradually decreased in frequency to less than 1 min$^{-1}$ after around 6 h of cumulative operation. This was also observed when operating the Gen. I neutron generator after the system had been vented and was attributed to impurities and micro protrusions on the surfaces inside the vacuum system which were removed in each breakdown process. Thus, over time the neutron generator system was “self-conditioning” in this way.

![Graph](image_url)

**Figure 4.30:** Loading of the fresh, deuterium-free target of the Gen. II neutron generator

The dashed lines separate consecutive days of loading.

Loading of the target was considered complete after around 19 h of cumulative operation. This was comparable to the previously observed 20 h in loading the fresh, deuterium-free target of the Gen. I neutron generator (see Section 2.4.1). However, during the loading of the beam target with deuterium ions supplied by the ECR microwave ion source, the high voltage and the beam current were kept constant in contrast to varying both high voltage and duty factor of extraction and hence beam current with the RF-driven setup. The averaged current read by the instrument of the high voltage power supply fluctuated which was a consequence of the adjustment of the microwave frequency and the deuterium gas pressure inside the ion source chamber.
The pressure in the ECR ion source chamber could not be measured directly. However, as shown in Figure 4.10, a PKR 251 pressure gauge supplied by Pfeiffer Vacuum AG, Switzerland, was connected to the side of the copper aperture that separated the vacuum chamber from the microwave ion source. Figure 4.31 shows the averaged current read by the instrument of the high voltage power supply corrected for the leakage current following Equation 4.3 as a function of the pressure measured by this pressure gauge.

The lower the pressure, the higher was the averaged ion beam current. This dependency was approximately linear, as was also found in Waldmann and Ludewigt [128] who directly measured the pressure inside the ion source chamber. At pressures below $9 \times 10^{-6}$ mbar the microwave discharge became unstable that was attributed to low chances of ionizing collisions between electrons and deuterium gas and hence the plasma could not be sustained. Conversely, at higher pressures, the rate of collisions of electrons with deuterium gas particles was so high, that the electrons could not gain enough energy for ionization, thus the plasma density in the ion chamber decreased [128]. The dip in the current reading at a pressure of around $1.1 \times 10^{-5}$ mbar came from changes in

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**Figure 4.31:** Effect of pressure in the ion source on ion beam current and microwave ion source operation

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the microwave frequency that was automatically adjusted by the microwave generator unit.

### 4.4.2 Verification of Increased Neutron Output

The Gen. II neutron generator was described in terms of neutron output per unit beam power to compare performance with the Gen. I design. To measure this characteristic, the accelerating potential was varied from $-50$ to $-145$ kV. The ion beam current was not actively controlled, because the extraction electrode was removed. Figure 4.32 shows the neutron yield, accelerating potential, and averaged ion beam current measured by the instrument of the high voltage power supply corrected for the leakage current according to Figure 4.27.

![Figure 4.32: Neutron output of the Gen. II neutron generator for different accelerating potentials](image)

The neutron generator performed very stably (high voltage breakdowns occurred less than 0.1 min$^{-1}$), only at accelerating potentials beyond $-120$ kV high voltage breakdowns occurred at a frequency of more than 2 min$^{-1}$. In comparison to the Gen. I neutron generator, the high voltage limit of $-90$ kV was surpassed. The peak neutron output was around $6.8 \times 10^7$ s$^{-1}$, which is roughly 40% higher than the peak neutron output of $4.8 \times 10^7$ s$^{-1}$ that was achieved with the Gen. I neutron generator (see Section 2.4). Stable operation of the source was possible at high voltages up to $-120$ kV with neutron outputs of up to $6 \times 10^7$ s$^{-1}$, which is a factor of eight higher than what the Gen. I neutron generator design with a stationary titanium target achieved.
Chapter 4. *Generation II Compact D-D Neutron Generator at PSI*

The total neutron output and neutron yield per unit beam power are shown in Figures 4.33 and 4.34 and the fraction of estimated neutron output to the theoretically expected one from Equation 1.8 is shown in Figure 4.35. There is no evidence of out-gassing of deuterium (as would be the case if the ratios were to drop for an increase in beam power). In comparison with the Gen. I neutron generator, the neutron yield per unit beam power was higher and linearly increased with the beam power in the Gen. II neutron generator. However, it must be kept in mind that for the measurements with the Gen. I neutron generator the averaged target current values were not corrected for any leakage current. On top of that during those measurements the accelerating potential was kept constant and the duty factor of extraction adjusted to change the ion beam current and hence vary the beam power. This was the opposite as during the measurements with the Gen. II design.

The offset between actual and theoretical neutron yield still remains in the Gen. II neutron generator. Reasons can be found as discussed for the Gen. I neutron generator in the approximation of the thick-target yield estimation (e.g. the deuterium density in the target less than two) as well as uncertainties in the MCNP6 model and reading of the LB6411 neutron probe. Also, there can be a “loss” of ion beam current when ions get neutralized by collisions with neutrals in the accelerator column, or the actual beam current can be overestimated by a non-zero contribution of secondary back-streaming electrons as they are likely not perfectly suppressed. Lastly, contributions of non-mono-atomic ion species in the ion beam can lead to an offset between measured and expected neutron yield.
Figure 4.34: Comparison of neutron output per unit beam power between Gen. I and Gen. II neutron generator design

The results in Adams et al. [60] were reported with the Gen. I neutron generator with a stationary target.

Figure 4.35: Comparison of fraction of estimated to expected total neutron yield between the Gen. I and Gen. II neutron generator design

The results in Adams et al. [60] were reported with the Gen. I neutron generator with a stationary target.

The results show that the Gen. II neutron generator can operate stably with higher neutron yields than the Gen. I neutron generator. This is attributed to the improvements of the neutron generator housing, adoption of the ECR microwave ion source, and reduction of secondary backstreaming electrons with the electron suppression electrode which result in fewer high voltage breakdowns.
4.4.3 Emitting Spot Size Measurement

The emitting spot size of the Gen. II neutron generator was determined with the technique developed in Section 3.2. During the attenuating edge experiment, the electron suppression electrode was biased to $-100$ kV (with $1.4$ kV bias towards the beam target) with an averaged ion beam current read by the instrument of the target high voltage power supply and corrected for the leakage current of around $0.5$ mA. The $20$ mm thick tungsten attenuating edge was placed at a distance of $10$ mm from the outer surface of the vacuum chamber and moved perpendicular to the path between a scintillator and the neutron emitting spot. The scintillator was placed $63$ cm from the neutron spot. The measurement layout was analogous to the one sketched in Figure 3.15. Treatment of the response of the detector to the movement of the tungsten edge was the same as described in detail in Section 3.2. MCNP6 was used to create a lookup table for the attenuating edge measurement with the Gen. II neutron generator geometry for Gaussian and uniform disc neutron source definitions. This lookup table is shown in Figure 4.36.

![Figure 4.36: Lookup table relating the measured FWHM in the detector to the source diameter of the Gen. II neutron generator](image)

The lookup table values differed less than $1\%$ from the one for the Gen. I neutron generator because the dimensions in the attenuating edge experiment have changed only slightly. Figure 4.37 shows the edge spread function (ESF) normalized to the averaged values when the edge was moved fully in the path between the detector and the neutron spot. The errors in Figure 4.37 came from Gaussian error propagation from the statistical counting uncertainties in the reference detectors used for neutron flux normalization.
and from statistical counting uncertainties in the detector that measured the neutron intensity variation in response to the movement of the tungsten edge. A logistic function (from Equation 3.2) was fitted 1000 times to the ESF as described in Section 3.2. In this way, the FWHM seen by the detector was determined to $1.5 \pm 0.2$ mm, where the error stems from the standard deviation of the distribution of the 1000 FWHMs found from the logistic fits (as described in Section 3.2).

For the measured FWHM in the detector of 1.5 mm, this results in an extent of the top-hat distributed neutron emitting spot of 2.6 mm. As outlined in Section 3.2, the neutron emitting spot size does not have to be the same as the shape of the ion spatial distribution on the target surface that is shown in Figure 4.3 for the Gen. II neutron generator. Because the argument can be made that the spot shape in case of the Gen. II neutron generator is closer to a top-hat profile than a Gaussian, the lookup table from the MCNP6 simulation to be used for the spot size determination could be closer to the uniform disc one.

![Figure 4.37: Gen. II neutron generator emitting spot size measurement](image)

The FWHM seen by the detector from the logistic fit was $1.5 \pm 0.2$ mm.

Table 4.1 summarizes the determination of the emitting spot size using Gaussian and uniform source definitions. From this investigation, the conclusion is that the spot size falls within the range of 1.7 to 2.6 mm and is smaller compared to the emitting spot size of the Gen. I neutron generator design that was determined to be between 3 and 4 mm.
<table>
<thead>
<tr>
<th>FWHM seen by the detector [mm]</th>
<th>Emitting spot FWHM (Gaussian) [mm]</th>
<th>Emitting spot FWHM (top-hat) [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.5 \pm 0.2$</td>
<td>$1.7 \pm 0.2$</td>
<td>$2.6 \pm 0.3$</td>
</tr>
</tbody>
</table>

Table 4.1: Emitting spot size determination for the Gen. II neutron generator
Chapter 5

Conclusions and Future Work

In this work the following milestones were achieved:

- Design and implementation of a water-cooled, rotating beam target for a compact D-D fast neutron generator tailored for fast neutron imaging applications. CFD simulations were carried out to ensure that the maximum target temperature remained below the outgassing limit of deuterium in the titanium target. No signs of outgassing were observed from this target in any of the experiments in this work.

- Development of an accurate method to estimate the neutron output of a compact D-D fast neutron generator using thorough Monte Carlo simulations.

- Increase of neutron output at steady-state and stable conditions — i.e. high voltage breakdowns less than $0.1 \text{ min}^{-1}$ — in the Gen. I design of the PSI neutron generator by a factor of four, from $6.6 \times 10^6 \text{s}^{-1}$ to $2.9 \times 10^7 \text{s}^{-1}$.

- Improvement and application of an indirect neutron emitting spot measurement that verified the Gen. I neutron generator emitting spot size between 3 and 4 mm.

- Design and implementation of the Gen. II compact D-D fast neutron generator at PSI with a new housing, a new ECR microwave ion source, and an added electron suppression electrode. The high voltage limit was raised to up to $-145 \text{kV}$ where a peak neutron yield of $6.8 \times 10^7 \text{s}^{-1}$ was achieved. Stable operation was possible at up to $-120 \text{kV}$ with neutron yields of up to $6 \times 10^7 \text{s}^{-1}$. This represents an increase in stable neutron yield of a factor of two compared to the Gen. I neutron generator with rotating target and an increase of almost a factor of eight compared to the original Gen. I neutron generator design with a stationary target. The neutron emitting spot size of the Gen. II neutron generator was found to be within a range of 1.7 to 2.6 mm.
The achievements with the Gen. II PSI compact D-D fast neutron generator represent a dramatic improvement in the usefulness of the device for radiation imaging or other applications. Figure 5.1 outlines how the Gen. II neutron generator design performs in comparison with commercially available sources, depicted in Figure 1.4. The time per radiograph (for the scenario outlined in Section 1.1.2) is comparable to or better than those of commercially available designs. This is with a neutron emitting spot size that is significantly smaller, which means a system which requires a smaller footprint and less biological shielding than a larger emitting spot and higher output alternative. Furthermore, the device has been thoroughly characterized and its small size and potential mobility in comparison with larger scale neutron sources, outlined in Section 1.1, make it extremely attractive for in-field applications or otherwise where a mobile source is required.

Further increases in the neutron output of the Gen. II neutron generator design could be realized by switching from the D-D to the D-T neutron producing reaction, which can for example be achieved by using a mixed D-T gas to feed the ion source. This switch would increase the neutron output because the reaction cross section for the D-T reaction is around two orders of magnitude higher than the D-D reaction in the typical energy range in which a compact fast neutron generator operates (see Figure 1.2). With an equal mix of deuterium and tritium, this means roughly a 50 times higher overall

![Figure 5.1: Time per radiograph for a range of neutron outputs (D-D) and emitting spot sizes](image-url)

Evolution of the estimated time per radiograph for the compact D-D fast neutron generator optimized in this work in comparison with commercial sources.
output. The handling of radioactive tritium would, however, require very demanding practical considerations due to its hazards. Such a change would also mean that neutrons with a center of mass energy of 2.45 MeV (from D-D) and 14.1 MeV (from D-T) would be produced with a roughly 1 to 100 ratio according to the respective reaction cross section in the energy range of interest (see Figure 1.2). For the application of imaging, this has the added benefit of imaging at two energies at the same time (at one given neutron emission angle) if energy-discrimination on the detector side can be employed.

A higher neutron output could also be achieved when increasing the accelerating potential and hence the energy of the deuterium ions impinging on the target. Figure 1.2 shows that the D-D fusion reaction cross section scales exponentially with increase in bombarding ion energy. High voltage breakdowns are the limiting factor of an increase in accelerating potential in the developed Gen. II neutron generator. This could be addressed by careful surface treatment (e.g. polishing, baking out of materials) and a switch to a more powerful turbomolecular pump. In addition, the deuterium gas flow can be optimized, as to reduce the pressure in the accelerator column thus limiting probability for high voltage breakdowns. It might be possible to maintain a deuterium plasma in the ion source at a lower gas flow rate when adopting a (solenoid) magnetic field modifying coil as outlined in Baumgarten et al. [130]. A reintroduction of the pulsed extraction electrode could also lead to enhanced stability of operation at higher accelerating potentials by limiting the ion beam current and thus presence of primary charged particles in the accelerator column. That has the added benefit of allowing a further decrease in the neutron emitting spot size in optimizing position, geometry, and bias voltage of the extraction electrode (see Figure 4.11). Apart of raising the energy of the ion beam, the ion beam current could also be increased to boost the neutron output. The neutron output (estimated for a thick-target from Equation 1.8) increases linearly with the ion beam current. As shown by Waldmann and Ludewigt [127], the extracted ion beam density scales well with the microwave power. They found that raising the ion beam current density increased by 30 % when the microwave power was increased from 200 to 400 W. This motivates investigation of performance with a microwave generator unit that offers output powers beyond the 200 W used in this work. Ultimately to maximize neutron output an overall optimum should be sought, where the highest acceleration voltage and beam power is reached which is still within the limits of target overheating at a given emitting spot size. Many steps were taken towards this optimum in this work, but the ones listed here represent potential future work to bring the performance closer to that overall optimum.

Reduction in the neutron emitting spot size, tremendously useful for imaging applications, can be achieved in the case of fan-beam tomography by rotating the orientation of
the target rod from a $z$ orientation to a $y$ orientation (assuming the same detector position). Then, a narrow slit ion source aperture could be adopted, where the slit extends in $y$ direction. Deuterons would be extracted through the narrow slit and hit the target surface along the direction of the symmetry line (in $y$ orientation). A detector placed at the 90° neutron emission angle would “see” direct neutrons emitted along the short edge of the emission spot. Figure 5.2 sketches this imaging setup. That would greatly increase neutron output (due to the overall larger spot size) but keep the emitting spot seen by the detector small. Such a system can be achieved with some effort from the developed Gen. II neutron generator design, requiring redesign of the vacuum chamber, rotating aluminum target structure, and electrical insulation of it. When designing this setup, the temperature limits of the titanium must be considered, as well as the ion beam optics, vacuum conditions, and current limitation of the high voltage power supply unit. Most importantly the gain in neutron output should be estimated, because from the kinetics of the D-D reaction the angular neutron yield is lowest at 90° emission angle (see Figure 1.6).

![Figure 5.2: Schematics of a proposed imaging setup using a horizontal slit aperture](image)

The beam target is oriented at 90° angle with respect to the directions of the deuterium ion beam. In this configuration the neutron output can be enhanced while keeping the neutron emitting spot in direction seen by the detector small.

For applications other than fast neutron imaging where high neutron fluxes are desired — e.g. activation experiments described in Ayllon et al. [42] — the Gen. II neutron
generator could be easily modified. The developed rotating beam target rod allows placement of a sample inside the hollow part (12 mm diameter) of the beam target (see for example Figure 2.15) and hence benefit from high neutron fluxes close to the birthplace of the neutrons. For such experiments where emitting spot size is less of a concern, the 1 mm aperture separating ion source and steel vacuum chamber can be exchanged for one with a larger diameter which can increase extractable ion beam density thus leading to a higher neutron output. Additionally, the beam power would be spread over a larger area on the target surface, making outgassing due to local target overheating less of a concern when the beam power increases.

Apart of these possibilities for further development of the compact D-D fast neutron generator at PSI, the device is already now extremely useful for fast neutron imaging applications, such as energy-selective transmission imaging described by Soubelet [43], or detector characterization efforts. With the earlier outlined decline in the number of large scale neutron imaging facilities, powerful compact neutron generators such as the one optimized in this work can contribute in providing means of keeping scientific and industrial endeavours running.
Appendix A

Titanium Coating Thickness Measurement

The thickness of the titanium coating on the proposed target rod was estimated using optical microscopy at PSI. Results in Figure A.1 and A.2 are additional measurements on the same piece that was cut off from the coated rod as detailed in Figure 2.19. For further details, see Section 2.3.3.

Figure A.1: Optical microscopy measurements
Samples for measurement of the titanium coating thickness were taken far away from the beam spot at the upper edge of the lower part of the target.
Figure A.2: Optical microscopy measurements

Samples for measurement of the titanium coating thickness were taken far away from the beam spot at the upper edge of the lower part of the target.
Appendix B

Extraction Electrode Failure in Generation II Neutron Generator

First tests of operation of the Generation II neutron generator without the electron suppression electrode showed very low stability of operation. Following many high voltage breakdowns (more than 1 min$^{-1}$) at moderate high voltage levels of $-80$ to $-120$ kV equipment failed regularly, e.g. the unit controlling the turbomolecular pump was damaged twice during these experiments. During this operation the target was biased to around $-90$ to $-100$ kV accelerating potential and the averaged target current read by the instrument of the high voltage power supply was 0.1 to 0.2 mA. The extraction electrode was biased to $-3$ kV and pulsed at a frequency of 3 kHz with 10 to 80% duty factor. The microwave generator operated at a forward set point power of 200 W and a frequency of 2.44 to 2.45 GHz. The frequency was optimized automatically by the microwave generator to minimize reflected power which ranged between 5 and 12 W. The neutron ambient dose rate measured with the LB6411 neutron probe was below 30 pSv h$^{-1}$ which was below the limit where the LB112 dose rate monitor was calibrated to output a current proportional to the neutron dose rate. This made estimation of neutron output using the LB6411 neutron probe not possible, but it was well below $1 \times 10^6$ s$^{-1}$. Upon inspection after around cumulative 8 h of operation the MACOR insulator facing the beam target was found to be burnt as shown in Figure B.1. The burnt spot originated likely from bombardment with secondary backstreaming electrons, which also contributed to the frequent high voltage breakdowns by releasing particles from the MACOR. The formerly white zirconia screws were discolored yellowish, which was an indication of overheating of the extraction electrode assembly due to the low thermal conductivity of $1.5$ W m$^{-1}$ kg$^{-1}$ of the (ceramic) MACOR material [124].

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Appendix B. Extraction Electrode Failure in Generation II Neutron Generator

Figure B.1: Photograph of the burnt spot on the MACOR insulator facing the beam target

B.1 Performance after Removal of Extraction Electrode

After removal of the extraction electrode assembly the neutron generator operated more stably without damage to any devices connected to or near the neutron generator. Figure B.2 shows the performance without extraction electrode at a target negative high voltage of $-90$ to $-100$ kV and microwave forward power of 200 W with between 6 and 10 W reflected power at a microwave frequency of 2.44 to 2.45 GHz.

![Figure B.2: Performance of the Gen. II neutron generator operation](image)

(a) Measurement day 1.  (b) Measurement day 2.

The previously observed failures of equipment did not occur during these measurements. However, the averaged target current measured with the high voltage power supply frequently, around 1 to 2 min$^{-1}$, rose and reached 2 mA which was the maximum the high voltage power supply could handle and hence shut off the high voltage supply internally.
to prevent damage to the unit. The estimated neutron output was steadily increasing to a maximum of around $1.5 \times 10^7 \text{s}^{-1}$ during these measurements. The increase in neutron yield was attributed to the loading phase when the fresh, deuterium-free target was continually loaded with deuterium, thus increasing the deuterium density in the target. This behaviour was also observed in the Gen. I design when loading a fresh, deuterium-free spot on the titanium target with deuterium as outlined for example in Figure 2.21. During the around 9 h total measurement window, the high voltage power supply stopped following a series of high voltage breakdowns after around 30 min of operation and after around 60 min, on the respective measurement day.
Bibliography


Bibliography


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References
- Available upon request

Zürich, April 20, 2020
List of Publications


