

Determination of hydrogen content and its influence on neutron shielding properties of concrete designed for IFMIF-DONES

Tomasz Piotrowski^{a, b}, Maja Kepniak^{a, *}, Elżbieta Horszczaruk^b,
Maria Jose Martinez-Echevarria^{c, d}, Rafał Michalczyk^{a, d}, Armando Arvizu-Montes^{c, d},
Łukasz Ciupiński^a, Santiago Becerril Jarque^d, Kazimierz Józefiak^{a, d}, Yuefeng Qiu^e,
Martin Ansorge^f, Hari Chohan^g, Magdalena Grodkowska^a

^a Warsaw University of Technology, Warsaw, Poland

^b West Pomeranian University of Technology in Szczecin, Szczecin, Poland

^c University of Granada, Granada, Spain

^d IFMIF-DONES España, Granada, Spain

^e Karlsruhe Institute of Technology, Karlsruhe, Germany

^f Nuclear Physics Institute of the Czech Academy of Sciences, Řež, Czech Republic

^g United Kingdom Atomic Energy Authority, Culham Centre for Fusion Energy, Oxon, UK

ARTICLE INFO

Keywords:

IFMIF-DONES
Radiation
Attenuation
Neutron
Concrete
Magnetite

ABSTRACT

Neutron shielding efficiency is mainly related to atomic composition of composites like concrete. Fast neutron attenuation is primarily governed by neutron moderation through light elements, particularly hydrogen, whereas thermal neutron absorption depends on the absorption characteristics of individual nuclei. In this paper the measurements by different methods of hydrogen content in ordinary dolomite concrete OC and heavy-weight magnetite concrete MC designed for International Fusion Materials Irradiation Facility – DEMO-Oriented Neutron Source (IFMIF-DONES) have been presented. Based on the results, neutron shielding parameters were calculated and compared with those of concretes developed for ITER, an international fusion energy research project. The results showed that the relative hydrogen content in MC was lower than in OC. However, the higher density and increased iron (Fe) content resulting from the use of magnetite aggregate yielded more favorable neutron-shielding characteristics for MC. The results also indicate that the optimized IFMIF-DONES concretes offer improved neutron shielding potential compared with the reference ITER concretes.

1. Introduction

The composition of the investigated concretes was developed on the basis of the reference ordinary dolomite aggregate concrete designed for ITER, an international fusion energy research project, and subsequently optimized for the International Fusion Materials Irradiation Facility – DEMO-Oriented Neutron Source (IFMIF-DONES) [1–3]. Optimized composition allowed for the preparation of ordinary dolomite aggregate OC and heavyweight magnetite concrete MC characterized by better technical and shielding properties than the references [4]. In this investigation the assumption was that water in 20% of the cement mass is chemically bound water taken into account in the calculation of neutron shielding efficiency [4]. At the same time the references on chemical (atomic) composition [2,3] in ITER documentation show the

possibility of determination of hydrogen content by two different methods: by measurement in a thermal conductivity detector after sample burning and separation of combustion gases through a chromatographic column (called direct measurement), or by estimation from bound water determined by thermogravimetric analysis (called TGA). The conclusion from the comparison was that the measured and calculated values of hydrogen and carbon are very close to one another, with small differences observed between the measured and calculated values of hydrogen, but these values are comparable anyway. Nevertheless, the recommended normalized data for chemical composition of concrete to be used in the MCNP models of DONES is based on direct measurement.

The accurate determination of hydrogen content is of particular importance for the design and analysis of shielding materials intended for fusion facilities. While numerous studies have focused on the

* Corresponding author.

E-mail address: maja.kepniak@pw.edu.pl (M. Kepniak).

<https://doi.org/10.1016/j.conbuildmat.2026.148298>

Received 23 March 2026; Received in revised form 29 June 2026; Accepted 20 September 2026

Available online 28 September 2026

0950-0618/© 2026 The Author(s). Published by Elsevier Ltd. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

influence of density, aggregate type and elemental composition on shielding performance, relatively limited attention has been devoted to the influence of hydrogen determination methodology on the results of neutronic calculations and shielding assessments.

The importance of hydrogen in neutron shielding analysis cannot be overstated. It is because neutrons have no charge and can interact with the nuclei of a target atom only. The range of a neutron is dependent on its initial energy. Fast neutrons with energy of over 1 MeV practically cannot be absorbed so they have to be attenuated first by scattering – elastic or inelastic.

Inelastic scattering is more prevalent for heavy nuclei and takes place when the neutron and the nuclei coalesce to form a compound nucleus, followed by the emission of a neutron with lower energy and a gamma ray.

Fast neutron attenuation is therefore governed primarily by neutron moderation through elastic scattering on light elements, particularly hydrogen. Following moderation, thermal neutrons may be absorbed by selected nuclei depending on their neutron absorption cross-sections. Unlike neutron moderation, thermal neutron absorption cannot be directly correlated with atomic number and depends on the nuclear characteristics of individual elements.

Heavyweight aggregates rich in iron are frequently used in shielding concrete because they attenuate neutrons through scattering and absorption and provide excellent gamma-ray shielding due to their high density. However, neutron interactions with iron can also generate secondary gamma radiation and activation products, which should be considered in shielding design.

1.1. Hydrogen content – shielding (literature review)

Hydrogen's unique properties make it indispensable for developing advanced shielding solutions, providing essential protection in environments where ionizing radiation is a significant concern [5].

Hydrogen is a highly effective material for shielding against ionizing radiation, largely due to its unique atomic properties. With an atomic number of 1 ($Z = 1$), hydrogen is exceptionally efficient at scattering neutrons and other forms of radiation [6]. This effectiveness stems from the fact that hydrogen's atomic mass is close to that of a neutron, enabling it to significantly reduce neutron energy through elastic collisions [7]. Each collision between a neutron and a hydrogen atom results in a substantial energy loss for the neutron, making hydrogen particularly valuable in radiation shielding.

In addition to its use in pure forms, hydrogen is also incorporated into composites and protective coatings [8,9]. Materials with a high hydrogen content, such as specific polymers and organic compounds, are highly prized for their radiation protection capabilities [10]. These applications leverage hydrogen's ability to absorb and scatter radiation energy, making it a critical component in modern shielding materials used across various industries, including the nuclear sector and space exploration [11]. Hydrogen's high ratio of atomic number to atomic mass further enhances its effectiveness as a shielding material [12]. In the fabrication of polymer nanocomposites used for shielding, hydrogen plays a crucial role, especially in neutron shielding [13,14]. Light atoms, such as those found in hydrogenous materials, are particularly effective at moderating fast and intermediate neutrons, as they slow down neutrons through elastic scattering [10].

1.2. Research gap, novelty and objectives

Previous studies have shown that the shielding performance of cementitious composites is governed not only by material density, but also by aggregate composition, elemental composition and microstructural compactness. Heavyweight aggregates such as barite and magnetite are commonly incorporated to enhance radiation attenuation, while recent research has also emphasized the need to combine shielding efficiency with sustainability-related aspects in the design of advanced

cementitious and geopolymer-based materials [15,16].

Although hydrogen is widely recognized as one of the most important elements governing neutron moderation in shielding materials, limited information is available regarding the consistency and reliability of different hydrogen determination methods applied to cement-based shielding concretes. Existing studies have primarily focused on shielding performance, density optimization and material composition, whereas comparatively little attention has been devoted to the influence of hydrogen quantification methodology on the results of neutronic calculations. Furthermore, the uncertainties associated with different experimental approaches and their potential impact on the assessment of neutron shielding parameters remain insufficiently investigated.

Therefore, the novelty of this study lies in the comparative evaluation of different hydrogen determination approaches for cement-based shielding materials intended for fusion applications. Particular attention is given to the consistency of the obtained results and to the influence of hydrogen content on calculated neutron shielding parameters. By combining experimental characterization with neutron shielding calculations, this work provides new insight into the reliability of hydrogen quantification and its significance for the design and assessment of shielding structures for IFMIF-DONES.

Therefore, the objectives of this study were: (i) to determine the hydrogen content of selected cement-based shielding materials using different experimental approaches; (ii) to compare the obtained results and evaluate the sources of discrepancies between determination methods; (iii) to assess the influence of hydrogen content on calculated neutron shielding parameters; and (iv) to provide recommendations regarding the applicability of hydrogen determination methods for neutronic calculations and shielding design in fusion facilities.

2. Materials and methods

2.1. Evaluation of neutron radiation shielding efficiency

Dependence of fast neutron attenuation on hydrogen content described above has its expression in calculation of fast neutron effective removal cross-sections method. The classical gamma-ray mass attenuation coefficient is presented only as a reference framework illustrating the analogy between photon attenuation and neutron removal approaches. In the present study, Eq. (1) is not used directly in the calculations but serves to introduce the neutron removal cross-section methodology presented in Eq. (2).

$$\mu/\rho = \sum_i w_i \cdot (\mu/\rho)_i \quad (1)$$

but the linear attenuation coefficient, μ is replaced by the fast neutron removal linear coefficient (called the fast neutron removal cross-section), Σ_R . (2):

$$\Sigma_R/\rho = \sum_i w_i \cdot (\Sigma_R/\rho)_i \quad (2)$$

where:

w_i – weight fraction of i^{th} constituent,

$(\Sigma_R/\rho)_i$ – fast neutron mass removal coefficient of i^{th} constituent

Weight fraction, w_i is proportional to partial density, W_i by its density according to Eq. (3)

$$W_i = w_i \cdot \rho_s \quad (3)$$

where:

ρ_s – specific density

As it was said that the fast neutron mass removal cross-section by elastic scattering varies smoothly with the atomic weight so its value can be calculated using the empirical equations related to the atomic mass A or atomic number Z of the element presented by Wood [17]:

$$\Sigma_R/\rho = 0.21 \cdot A^{-0.56}; A \leq 12 \quad (4)$$

$$\Sigma_R/\rho = 0.00662 \bullet A^{-1/3} + 0.33 \bullet A^{-2/3} - 0.221 \bullet A^{-1}; A > 12 \quad (5)$$

$$\Sigma_R/\rho = 0.190 \bullet Z^{-0.743}; Z \leq 8 \quad (6)$$

$$\Sigma_R/\rho = 0.125 \bullet Z^{-0.565}; Z > 8 \quad (7)$$

or by Chilton [18]:

$$\Sigma_R/\rho = 0.0206 \bullet A^{-1/3} \bullet Z^{-0.294} \quad (8)$$

Most of the values of the fast neutron mass removal cross-sections for elements and some compounds have been experimentally and computationally verified and published [18–21]. This method is the core of software like MERCSEF-N [22], WinNC [23] ParShield [24] and is used by many researchers for neutron shielding efficiency evaluation.

To summarize, the fast neutron effective removal cross section value Σ_R is more like a linear attenuation coefficient given in cm^{-1} , not like a cross-section commonly given in cm^2 . It is finally calculated by Eq. (9)

$$\Sigma_R = \sum_i W_i \bullet (\Sigma_R/\rho)_i \quad (9)$$

It is described as the probability that a fast energy neutron undergoes an interaction on the first collision, which removes it from the group of penetrating, uncollided neutrons.

Generally, this approach is based on the presence of hydrogen. In materials such as concrete containing sufficient hydrogen, neutron attenuation is dominated by the removal process associated with neutron moderation. It should be noted that the effective removal cross-section Σ_R remains relatively stable for neutron energies between 2 and 12 MeV [19]. However, local deviations have been reported for specific energy intervals. For example, in the 6–8 MeV range, the observed value of Σ_R is approximately two-thirds of the total neutron cross-section Σ_t [25], where Σ_t represents the combined contribution of elastic scattering, inelastic scattering and absorption processes. In order to evaluate materials regarding neutron shielding efficiency distinguishing different attenuation and absorption phenomena a method based on macroscopic cross-sections for a different interaction is proposed [26]. Here instead of fast neutron removal cross-sections, it uses a database of neutron scattering lengths and cross-sections that includes the thermal neutron microscopic cross-section as well. The values have been published by Sears [27] and adopted by the NIST Center for Neutron Research [28]. In this method the values of the microscopic cross-sections (bound scattering cross-sections σ_s ; coherent σ_{cs} and incoherent σ_{is} , and the absorption cross-section σ_a) are placed into simple Eq. for the mass attenuation coefficient:

$$\mu/\rho = \frac{N_A}{A} \bullet \sigma_i \quad (10)$$

and the specific neutron mass attenuation coefficient for a specific interaction is calculated according to Eq.

$$\Sigma_j/\rho = \frac{N_A}{A} \bullet \sigma_j \quad (11)$$

where:

$$N_A = 1.66 \cdot 10^{-24} \text{ g}$$

σ_i – microscopic cross-section for a specific interaction (j): scattering σ_s , (incoherent σ_{is} , coherent σ_{cs}) and absorption σ_a

Σ_j/ρ – neutron mass attenuation coefficient for a specific interaction (j); s - scattering, a - absorption

2.2. Description of samples

There have been prepared samples made of concrete, cement mortar and cement paste. Ordinary dolomite concrete (OC) has been designed

and optimized based on prescribed ITER OC. Following the ITER reference the magnetite aggregate has been used as well magnetite concrete (MC) has been prepared. Due to requirements regarding the consistency and relatively low water/cement (w/c) ratio a new-generation polycarboxylate superplasticizer has been used. Moreover, in order to eliminate the segregation possibility, the viscosity modifying admixture has been added as well. Detailed composition (Table 1) has been already published in 2024 by Piotrowski et al. [4] and as it has been described dolomite and magnetite aggregate granulometry optimization allowed for an increase in total aggregate content up to 2000 kg/m^3 for OC and 3571 kg/m^3 MC which resulted in higher density and better technical properties than the reference ITER concretes (Table 2).

In addition, the specimens made of cement mortar (marked as OM and MM) and cement paste (CP) have been prepared. The composition of mortar is the same as for the concrete but without coarse aggregates and cement paste is without both coarse and fine aggregate as well. Due to the visible difference between the light-coloured outer layer and the darker inner core of the cement paste specimen (CP), both regions were analysed separately. The colour contrast was most likely associated with differences in carbonation degree, moisture transport and local hydration conditions occurring during curing and storage. Since these factors may influence both hydrogen content and thermal decomposition behaviour, separate analyses were performed for the outer layer and the core.

2.3. Hydrogen content estimation, measurement and calculation

As it was described before hydrogen content in concrete can be estimated or measured. In the recent experimental studies [29] it has been concluded that there is no clear relation between neutron shielding efficiency and bound water content. For standard concrete based on silica and magnetite aggregate, more influential are cement and aggregate type and their atomic composition. Such statement led to the simple assumption of considering chemically bound water as 20% in relation to cement mass. It is twice as high as the result of the measurement of chemically bound water for CEM III, but it takes into account that hydration in this type of cement takes more time than 28 days due to the presence of granulated blast furnace slag (GBFS). This assumption has been effectively used for comparison of modification of concretes [26, 30] and for preliminary evaluation of DONES concretes as well [4].

The most precise and reference method for hydrogen content is a direct method consisting of measurement in a thermal conductivity detector after sample burning and separation of combustion gases through a chromatographic column. In this research the hydrogen content analysis was performed using the LECO ONH 836 elemental analyzer.

Prior to elemental analysis, the specimens were crushed using a mechanical testing machine and subsequently ground in an agate mortar to a particle size below 1 μm in order to obtain a homogeneous material. In the case of the cement paste specimen, the outer layer and the inner core were separated before grinding and analysed independently. All powdered samples were dried at 105 °C prior to testing. Hydrogen content was determined using a LECO ONH 836 elemental analyser. A pre-weighed sample was placed in a graphite crucible and heated in a pulse furnace under a high-purity helium (6.0) atmosphere. The released gases were transported through the analytical system by the carrier gas. Hydrogen was oxidised to H_2O and quantified using NDIR detection cells. Instrument calibration was performed using certified reference materials: Eltra 99100–25, Alpha Ar649 and Leco 502–416–0663 (Table 3). Each sample was measured twice and the reported value corresponds to the average result.

Following ITER references and literature hydrogen can be also estimated from bounded water determined by thermogravimetric analysis. It is carried out under nitrogen atmosphere from 20 °C to 1000 °C on powder sample (< 125 μm). This technique allows following the mass variation of a sample depending on time and temperature. It is coupled

Table 1

Composition for ITER OC reference concrete and DONES investigated concretes (OC an MC).

ITER OC		DONES OC		DONES MC	
Composition [kg/m³]					
Total aggregate	1745	Total aggregate	2000	Total aggregate	3571
0/4 semi-crushed limestone sand	900	0/4 dolomite limestone	900	0/2 magnetite	357
4/16	350	4/8 dolomite limestone	200	0/8 magnetite	1607
rolled natural gravel					
11.2/22.4	445	6/12 dolomite limestone	800	0/20 magnetite	1607
rolled natural gravel					
Limestone fillers	50	11/22 dolomite limestone	100		
CEM I 52.5 N PM ES	240	CEM III/B 42.5 N-LH/SR	360	CEM III/B 42.5 N-LH/SR	360
GGBS	100				
Superplasticizer	3.12	Superplasticizer (Polycarboxylate)	2.88	Superplasticizer (Polycarboxylate)	2.88
(Acrylic)				Stabiliser	2.16
				(Strach based)	

Table 2

Technical properties for ITER OC reference concrete and DONES investigated concretes (OC an MC).

Properties	ITER OC	DONES OC	DONES MC
Density [g/cm ³]	2.289	2.507	3.938
Compressive strength [MPa] 28 days	54.0	76.4	79.0
Compressive strength [MPa] 90 days	59.0	79.3	79.9
Tensile strength [MPa] 28 days	4.54	3.85	4.34

Table 3

Standards used for calibration to determine the hydrogen content in sample.

Standard	Eltra 99100–25	Alpha Ar649	Leco 502–416-0663
H content	2,8 + -0,4 ppm	0,0193%	5,4 + -0,6 ppm

with DTA (Differential Thermal Analysis), which compares the differential thermal flow between the sample and an inert reference. Then, exothermic or endothermic changes in the sample are detected. The key issue in this method is a proper selection of temperature ranges determining: evaporation of free water (usually < 80–100°C), bound water evacuation from Ca(OH)₂ (usually between 80 and 100°C and 600–630°C) and decomposition of CaCO₃ with CO₂ emission (usually > 600–630°C). Masoud et al. [31] identified three weight losses stemming from the decomposition of calcium silicate hydrate (C–S–H gel) (75–180 °C), calcium hydroxide (CH) (410–465 °C), and calcite (C) (685–760 °C). Moreover, he implies the dehydroxylation of structural water (SW, chemically-bound water) of chrysotile aggregates related to the weight loss at the temperature range of 660–685 °C. Finally he determined water contents to be between 9.69% and 11.52%.

Table 4

Results of hydrogen content by direct measurement.

Sample	Specimen	H content [%]	Average H content [%]	SD [%]	COV [%]	Density [g/cm ³]	H content [g/cm ³]
CP – outer layer	01	2.360	2.370	0.014	0.6	1.86	0.0441
	02	2.380					
CP - core	01	2.230	2.320	0.127	5.5	1.86	0.0432
	02	2.410					
OM	01	0.485	0.498	0.018	3.6	2.49	0.0124
	02	0.510					
MM	01	0.332	0.322	0.014	4.3	3.76	0.0121
	02	0.312					
OC	01	0.351	0.350	0.002	0.6	2.53	0.0089
	02	0.348					
MC	01	0.307	0.302	0.008	2.6	3.82	0.0115
	02	0.296					

3. Results

3.1. Direct measurement of hydrogen content

Each specimen, dried at 105°C, was measured twice, and the results were averaged (Table 4) but despite the limited number of measurement results, they have very good statistics and the maximum coefficient of variation (COV) is only about 5.5% and standard deviation (SD) is only 0.127. Regarding the cement paste specimens, no significant difference in hydrogen content was observed between the outer layer and the core. Comparison of the mortar and concrete specimens indicates that the hydrogen content expressed as mass percentage was higher in the ordinary concrete (OC) than in the heavyweight magnetite concrete (MC). However, when normalized with respect to material density (g/cm³), the hydrogen content of MC became comparable to, or even higher than, that of OC. This observation suggests that magnetite concrete may provide improved fast neutron attenuation not only because of its iron-rich aggregate but also owing to its higher volumetric hydrogen content.

3.2. Hydrogen estimation using thermogravimetric analysis

Thermogravimetric analysis (TGA) coupled with mass spectrometry was performed using Netzsch STA 449 C (TG) and QGA Gas Analysis System, Hiden Analytical Ltd. (MS) equipment. Measurements were performed twice for each sample in a ceramic crucible. Samples used for measurement have been previously dried at 105°C; the mass of the tested sample was approximately 10 mg. Measurement parameters: range was 30–1000°C with temperature increase rate – 10 °C/min. Measurement atmosphere was nitrogen (30 ml/min) and argon (30 ml/min). Measurements were preceded by preparing a calibration curve for an empty crucible. During the measurement, the intensity of the MS signal of the exhaust gases was also measured. Two gases were indicated: $m/z = 18 - \text{H}_2\text{O}$ and $m/z = 44 - \text{CO}_2$.

In the conducted analysis, different temperature ranges were selected based on the reaction dynamics and the emission of carbon dioxide (CO_2) and water (H_2O). These ranges were chosen to obtain accurate results for hydrogen content in each of the analyzed samples. Consequently, the selected temperature ranges may differ from those used in similar published studies.

3.2.1. Cement paste

For the cement paste from the outer layer (CPouter, Figs. 1 and 2a) and the core (CPcore, Fig. 2b), different behaviors were observed. The CPouter sample underwent thermal decomposition with only water emission, as evidenced by the absence of peaks indicating CO_2 emission. Therefore, the hydrogen content was calculated using the total mass loss across the entire measurement range, which was 16.5%. In contrast, the CPcore sample exhibited a distinct CO_2 emission peak during thermal decomposition within the temperature range of 500–700°C. Since water was also emitted in this range, it was impossible to attribute the thermal decomposition to specific signals definitively. Despite this, the hydrogen content was calculated using the mass loss within the 30–500°C range, amounting to 13.1%.

3.2.2. Mortar

For ordinary mortar (Fig. 3a) and magnetite mortar (Fig. 3b), the main desorbing gas in the 600–1000°C range was CO_2 . Therefore, only the mass loss within the 30–600°C range was considered for hydrogen content calculation. This resulted in a H_2O mass loss of 0.71% for ordinary mortar and 1.44% for magnetite mortar (MM).

3.2.3. Concrete

The heavy magnetite concrete (MC, Fig. 4b) underwent thermal decomposition with water emission only, indicated by the lack of CO_2 emission peaks. The water content was calculated based on the total mass loss across the entire measurement range, which was 2.16%. Ordinary concrete (OC, Fig. 4a) also demonstrated CO_2 as the primary desorbing gas in the 600–1000°C range. Thus, only the mass loss in the 30–600°C range was considered for water content calculation, resulting in a loss of 0.87%.

Based on the TGA analyses, calculations related to the hydrogen

content in cement pastes, mortars, and concretes were performed (Table 5). The substantial differences observed between the thermogravimetric profiles of the investigated materials can be explained by differences in aggregate mineralogy rather than solely by the composition of the cementitious matrix. Although the mass of the analysed specimen was relatively small (approximately 10 mg), the ground material used for TG-MS analysis was previously homogenized by crushing and grinding to a particle size below 1 μm . Consequently, the analysed powder contained both cementitious phases and aggregate-derived mineral constituents.

The XRD results demonstrated that the ordinary concrete and mortar samples (OC and OM) were dominated by dolomite-containing phases, whereas the heavyweight concrete and mortar samples (MC and MM) contained predominantly magnetite, hematite and quartz. During heating, dolomite undergoes thermal decomposition accompanied by significant CO_2 release, which was clearly observed in the TG-MS results for OC and OM. In contrast, the magnetite-based materials did not contain comparable amounts of carbonate phases and therefore exhibited substantially different thermal decomposition behaviour.

These observations indicate that the differences in TG-MS profiles originate primarily from differences in mineral composition and decomposition mechanisms rather than from variations in cement hydration products alone. Therefore, despite the relatively small specimen mass used in the TG analysis, the influence of aggregate mineralogy remained significant and contributed to the observed differences between the investigated materials.

3.3. Calculation of atomic composition

Accurate determination of atomic composition is essential for reliable neutron shielding calculations, since macroscopic interaction cross-sections and fast neutron effective removal cross-sections depend directly on elemental mass fractions. Therefore, the chemical composition of the investigated materials was established using a combined methodology integrating experimental measurements with engineering-based hydration assumptions. The baseline elemental composition of cement and aggregates was derived from mix design data and reference chemical analyses of constituent materials. Mineralogical compositions

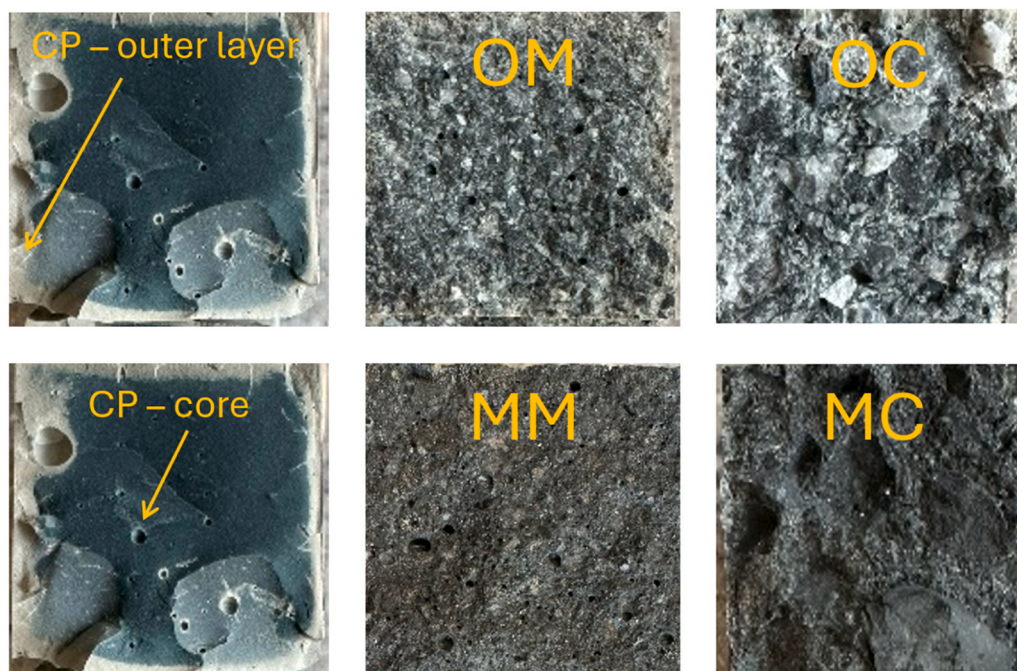


Fig. 1. Samples of cement paste CP, cement mortars (OC-M and MC-M) and concretes (OC and MC).

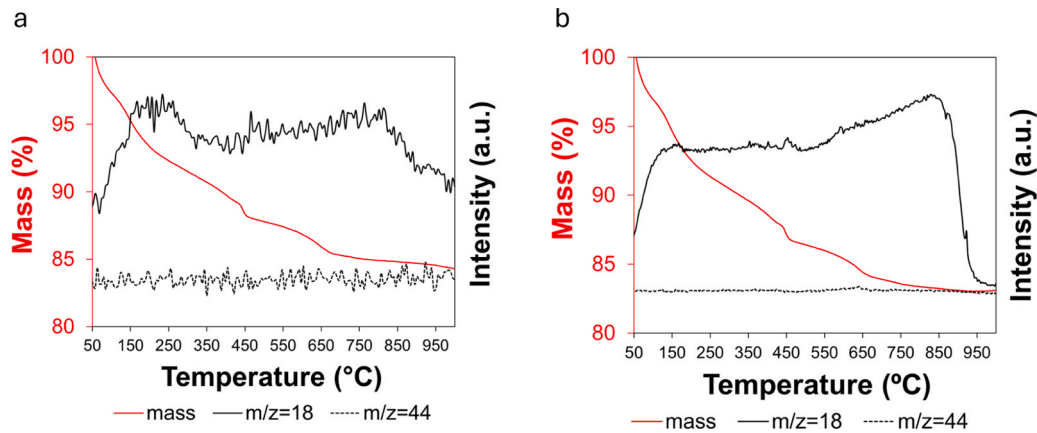


Fig. 2. Thermal decomposition profiles: a - cement paste outer layer (CPcover); b - cement paste from core (CPcore).

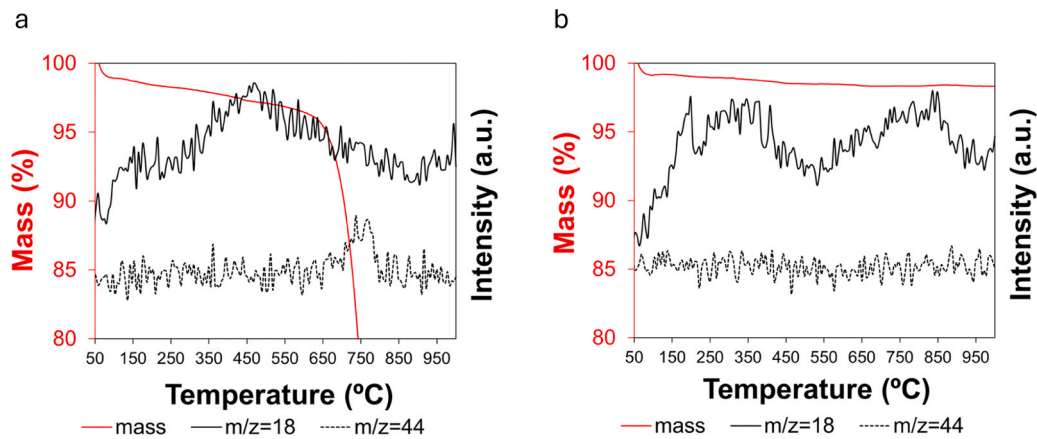


Fig. 3. Thermal decomposition profiles: a - ordinary mortar (OM); b - magnetite mortar (MM).

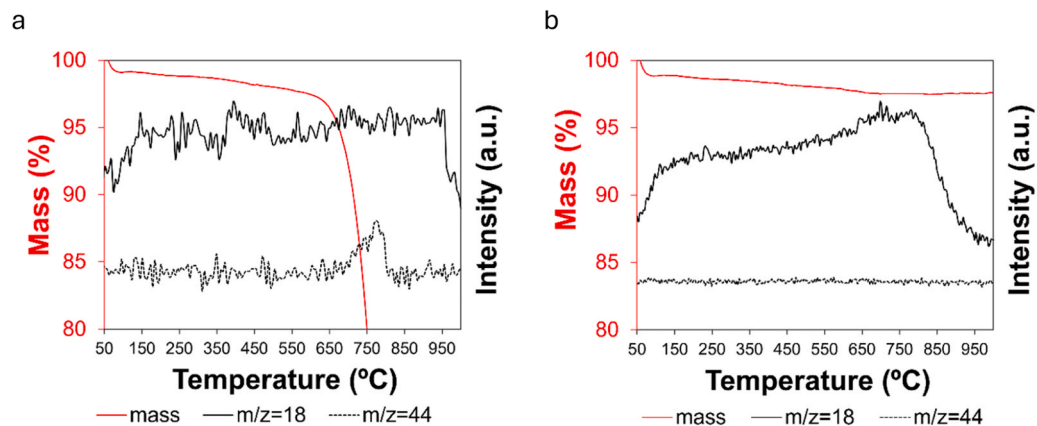


Fig. 4. Thermal decomposition profiles: a - ordinary dolomite concrete (OC); b - heavy magnetite concrete (MC).

of dolomite and magnetite aggregates were adopted consistently with previously published data for ITER and DONES shielding concretes, while the elemental composition of CEM III/B cement was introduced based on manufacturer specifications and literature values for blast furnace slag blended systems.

Particular attention was given to accurate determination of hydrogen content due to its dominant role in neutron moderation through elastic scattering interactions. Hydrogen mass fraction was primarily determined by direct elemental measurement using combustion analysis with thermal conductivity detection. This method provides direct

quantification of elemental hydrogen and was adopted as the reference input for normalization of the final atomic composition used in neutron shielding calculations. The experimentally determined hydrogen values were combined with the elemental composition of the remaining constituents, and the resulting elemental fractions were normalized to ensure that the total mass fraction equals unity.

In addition to direct measurement, an alternative engineering estimation was introduced based on assumed cement hydration degree. According to established cement hydration models, complete hydration of Portland cement requires approximately 0.23–0.25 g of chemically

Table 5
Results of hydrogen content by TGA.

Sample	Specimen	Mass loss - H ₂ O [%]	H content [%]	Average H content [%]	SD [%]	Density [g/cm ³]	H content [g/cm ³]
CP – outer layer	01	15.70	1.74	1.83	0.084	1.86	0.0340
	02	17.21	1.91				
CP - core	01	13.13	1.46	1.46	0.001	1.86	0.0272
	02	13.12	1.46				
OM	01	0.77	0.09	0.08	0.007	2.49	0.0020
	02	0.64	0.07				
MM	01	1.67	0.19	0.16	0.026	3.76	0.0060
	02	1.20	0.13				
OC	01	0.85	0.09	0.10	0.002	2.53	0.0025
	02	0.88	0.10				
MC	01	2.50	0.28	0.24	0.038	3.82	0.0092
	02	1.81	0.20				

bound water per gram of cement; however, full stoichiometric hydration is rarely achieved in practical concrete systems due to limitations associated with curing conditions, internal diffusion constraints, and progressive microstructural densification. This aspect is particularly relevant for blended cements such as CEM III/B, where hydration kinetics are slower and hydration may remain incomplete even at extended curing times. Therefore, instead of assuming full hydration, a realistic engineering approximation was adopted, in which chemically bound water accounts for approximately 20% of the cement mass. This assumption reflects typical hydration levels in mature cementitious systems and avoids overestimating hydrogen content. The assumed bound water was converted into elemental hydrogen fraction using stoichiometric relations between H₂O mass and hydrogen content and incorporated into the overall elemental balance for sensitivity analysis purposes.

Thermogravimetric analysis (TGA) coupled with mass spectrometry was performed as supplementary material characterization to evaluate thermal decomposition behavior and gas evolution during heating. However, TGA-derived hydrogen contents were not used as quantitative input for final atomic composition calculations. Accurate determination of chemically bound water using TGA in complex cementitious systems requires a strict and standardized definition of temperature intervals corresponding to specific dehydration reactions. In the present study, different temperature ranges had to be selected due to overlapping release of H₂O and CO₂ and differences in reaction dynamics among samples, which may introduce methodological variability and reduce comparability with standardized compositional datasets. Furthermore, overlapping thermal events, such as dehydration of hydration products and carbonate decomposition, may lead to ambiguity in distinguishing chemically bound water from other mass-loss mechanisms. Since neutron shielding calculations are highly sensitive to hydrogen content, the direct elemental measurement method was considered more robust and less dependent on the interpretation of thermal decomposition

stages. Consequently, TGA results were treated as qualitative support rather than as quantitative input for defining the normalized elemental composition used in shielding calculations.

The final normalized elemental compositions were subsequently used to calculate atomic number densities and macroscopic interaction cross-sections. Particular attention was given to elements governing neutron interaction mechanisms, including hydrogen, iron, oxygen, calcium, and silicon. Hydrogen primarily moderates neutrons via elastic scattering, whereas iron-rich phases in magnetite aggregates enhance inelastic scattering and thermal neutron absorption. The use of both measured hydrogen content and hydration-based estimates enabled the assessment of the sensitivity of neutron shielding parameters to uncertainties associated with bound-water assumptions.

The results are presented in [Table 6](#).

3.4. Evaluation of neutron shielding efficiency

The experimentally determined atomic compositions were used as input data for neutron shielding and activation calculations, allowing evaluation of shielding performance based on real material parameters, including hydrogen content and minor elemental contributions. The obtained compositions for ordinary dolomite concrete (OC) and heavyweight magnetite concrete (MC) were compared with reference ITER concrete compositions in order to assess differences resulting from optimized mix design and material selection for IFMIF-DONES applications.

Although measurement of selected trace element concentrations was initially planned, these analyses were not completed due to personnel and technical limitations within the cooperating laboratory. Nevertheless, a sensitivity study was conducted to evaluate the influence of key material parameters on neutron shielding performance. The analysis focused on variables expected to significantly affect neutron attenuation, namely hydrogen content, cement amount, and water-to-cement

Table 6
Elemental composition of investigated concretes depending on hydrogen determination method (mass fraction, %).

Element	OC DONES – Elemental analysis	OC DONES – Hydration estimation	OC ITER	MC DONES – Elemental analysis	MC DONES – Hydration estimation	MC ITER
H	0.3500	0.3290	0.3932	0.3020	0.1998	0.2132
C	10.2869	10.3070	5.8987	–	–	0.5075
O	49.6606	49.5839	48.9443	28.6001	28.0302	31.1619
Na	0.0000	0.0000	0.2522	0.1808	0.1826	0.1015
Mg	9.8671	9.8864	0.5665	0.2746	0.2772	0.4974
Al	0.7513	0.7528	1.4886	0.6895	0.6960	0.3959
Si	1.9907	1.9946	15.3765	2.5672	2.5914	2.2331
P	0.0040	0.0040	0.0278	0.4493	0.4536	0.1015
S	1.0693	1.0714	0.2499	0.1276	0.1288	0.0914
Cl	0.0220	0.0221	0.0133	0.0133	0.0134	0.0203
K	0.0564	0.0565	0.4066	0.1710	0.1726	0.2030
Ca	24.1597	24.2069	25.2309	4.6975	4.7419	5.3087

(w/c) ratio. The variability ranges were defined based on available literature and experimental results from previous stages of the project.

A Monte Carlo-based sensitivity analysis comprising 10^3 calculation cases was performed to evaluate the influence of material parameter variability on the calculated neutron shielding parameters. It should be noted that the term Monte Carlo in the present study refers to stochastic sampling of material composition parameters rather than neutron transport simulations. No transport calculations involving shielding geometry, neutron source definition or particle tracking were performed.

The analysis was based on repeated random sampling of the water-to-cement ratio, cement content and chemically bound water content within predefined ranges reflecting realistic variations encountered in concrete production. The investigated ranges included variations in the water-to-cement ratio of 0.44 ± 0.10 and in the cement content of 300–360 kg/m³, consistent with the requirements of European standard EN 206. Hydrogen content was introduced through chemically bound water, expressed as a percentage of cement mass, with an assumed variability of 20–30%, based on prior research findings. According to the 68–95–99.7 statistical rule, standard deviations were assumed as one quarter of the total parameter range, corresponding to values of 0.05 for w/c ratio, 15 kg/m³ for cement content, and 2.5% for bound water content. For each generated material composition, the corresponding elemental composition and neutron interaction parameters (Σ_R , Σ_s , Σ_a and Σ_t) were calculated. The obtained distributions were subsequently used to evaluate the sensitivity of shielding-related parameters to uncertainties associated with material composition.

The reference composition used as the baseline for isolated variability analysis corresponded to the designed OC and MC concretes with a w/c ratio equal to 0.44, cement content of 360 kg/m³, and chemically bound water equal to 20% of cement mass. The results indicate that the highest sensitivity of neutron shielding parameters is associated with variations in chemically bound water, which directly affects hydrogen content. Consequently, the largest variations were observed in the macroscopic neutron-scattering cross-sections and the total macroscopic attenuation cross-sections. This behavior is consistent with hydrogen's dominant role in neutron moderation via elastic scattering (Table 7).

Despite the relatively high sensitivity of neutron interaction parameters to hydrogen variability, the resulting changes in overall shielding efficiency remained limited. The maximum observed variation did not exceed approximately 9% for ordinary concrete and 6.5% for heavyweight magnetite concrete. The lower sensitivity of MC is attributed to its higher density and significant iron content, which provide additional mechanisms for neutron interactions and reduce dependence on hydrogen concentration alone.

These findings confirm that neutron transport calculations performed using the determined atomic compositions for OC and MC concretes are robust with respect to realistic material variability. Therefore, the provided compositions can be considered reliable input data for neutronic modelling and shielding design within the IFMIF-DONES project framework.

4. Discussion

Determination of the real hydrogen content in shielding concretes is inherently challenging because hydrogen is not a primary constituent of

the mineral skeleton but is introduced mainly through water (free and chemically bound) and, depending on the cement system and curing history, can vary in time and space. In addition, the numerical value of hydrogen used for neutronics strongly depends on the adopted determination method. Direct elemental analysis quantifies the total hydrogen in the tested material, whereas engineering estimation, based on an assumed degree of hydration, converts chemically bound water to hydrogen content via stoichiometric relations. Consequently, different approaches may yield noticeably different hydrogen mass fractions even for the same concrete.

Despite this methodological dependence, the present results show that the impact of hydrogen uncertainty on the overall shielding conclusions remains limited within realistic variability ranges. The sensitivity study (Monte Carlo, 10^3 cases) demonstrated that hydrogen-related variability (introduced through the chemically bound water assumption) produces the largest dispersion in neutron-scattering-related macroscopic parameters, as physically expected because hydrogen dominates elastic scattering and fast-neutron moderation. However, the resulting variation in global shielding performance remained moderate, not exceeding ~9% for OC and ~6.5% for MC across the investigated ranges of w/c ratio, cement content, and bound water content. This indicates that, for practical shield design, the use of measured atomic compositions (with hydrogen determined by elemental analysis) provides robust input data, and that conservative engineering assumptions about bound water mainly influence safety margins rather than changing the ranking or qualitative conclusions.

This observation is consistent with modelling outcomes reported by Prochoń and Piotrowski [29] who showed that bound water content varies with cement and aggregate type but does not translate into a clear, direct relationship between hydrogen input from bound water and neutron shielding efficiency. Their findings support the interpretation that, in cementitious composites, shielding performance is governed by the combined action of moderation (light elements, primarily H) and attenuation/absorption processes determined by the full elemental composition and density, rather than by bound water alone. The reduced sensitivity observed here for heavyweight magnetite concrete further supports this general mechanism: in MC, the dense, iron-rich aggregate provides additional interaction channels (e.g., inelastic scattering), thereby decreasing the relative importance of hydrogen-related variability compared with ordinary concrete.

Comparable conclusions can also be drawn from studies intentionally modifying “hydrogen loading” in concrete. Malkapur et al. [7] investigated latex modified concretes where hydrogen content was varied through mix parameters and polymer/cement ratio and reported measurable improvements in neutron shielding with increasing hydrogen concentration within feasible mix ranges. Importantly, these studies also imply that, while hydrogen enrichment can enhance moderation, the magnitude of the improvement is constrained by practical compositional limits and must be evaluated alongside other mix-driven changes (density, matrix composition, and secondary radiation effects). In other words, hydrogen is a strong lever, but within realistic design windows it rarely causes order-of-magnitude changes—consistent with the moderate sensitivity observed in the present work.

Finally, engineering assumptions similar to the adopted approach (e.g., using a fixed fraction of water as “bound” or “effective” for shielding

Table 7
Variability of neutron shielding properties for OC and heavy MC concrete determined by Monte Carlo method.

		OC			MC				
		w/c ratio	Cement content	Bound water	All	w/c ratio	Cement content	Bound water	All
Cross-section of efficient fast neutron removal	Σ_R	1,9%	0,4%	1,0%	2,1%	2,0%	0,6%	2,1%	2,2%
Macroscopic cross-section of neutron scattering	Σ_s	0,7%	2,6%	8,7%	8,9%	1,1%	1,5%	6,0%	6,5%
Macroscopic cross-section of thermal neutron absorption	Σ_a	1,4%	0,8%	2,5%	2,9%	2,3%	1,2%	2,5%	2,6%
Total macroscopic cross-section of neutron attenuation	Σ_T	0,9%	2,0%	7,0%	7,1%	1,3%	1,0%	4,8%	5,2%

calculations) have been applied in prior neutron shielding evaluations of concretes, particularly when the aim is to provide stable, standardized input for transport calculations rather than to reproduce local curing-dependent moisture states [32]. In this context, the present results provide an important practical message: although the absolute hydrogen content depends on the selected quantification route, the conclusions relevant to shield design (comparative performance of OC vs MC and robustness under realistic variability in mix parameters) remain stable.

In summary, the optimized IFMIF-DONES concretes exhibit shielding-relevant atomic compositions that can be reliably used in neutron transport calculations. Direct elemental analysis is recommended as the reference approach for defining hydrogen content in normalized material cards, while hydration-based estimation is best treated as a sensitivity scenario reflecting realistic uncertainty in chemically bound water. The study confirms that magnetite concrete's superiority over ordinary concrete for neutron shielding is maintained even when hydrogen content varies within realistic bounds, and that the predicted shielding efficiency is robust enough to support design calculations and safety factors for IFMIF-DONES concrete shields.

The present study is limited to computational evaluation of neutron shielding parameters based on experimentally determined elemental compositions. Experimental neutron transmission measurements will be considered in future studies to validate the calculated attenuation characteristics.

5. Conclusions

The present study evaluated different approaches for hydrogen determination in cement-based shielding materials designed for IFMIF-DONES and assessed their influence on neutron shielding calculations. Based on the obtained results, the following conclusions can be drawn:

1. Direct elemental analysis using the LECO ONH 836 analyzer provided the most reliable determination of hydrogen content and is recommended as the reference method for defining normalized elemental compositions used in neutronic calculations.
2. Hydrogen contents estimated from thermogravimetric analysis and engineering assumptions based on chemically bound water differed from directly measured values, demonstrating the sensitivity of hydrogen quantification to the adopted methodology.
3. The hydrogen content was higher in ordinary dolomite concrete (OC) than in heavyweight magnetite concrete (MC). However, due to the higher density and iron content of magnetite aggregate, MC exhibited more favourable neutron shielding characteristics.
4. The Monte Carlo sensitivity analysis showed that hydrogen-related variability had the strongest influence on neutron scattering parameters. Nevertheless, the resulting variability of the overall neutron shielding parameters remained limited, not exceeding approximately 9% for OC and 6.5% for MC.
5. The optimized IFMIF-DONES concretes exhibited shielding-relevant atomic compositions that can be reliably used in neutron shielding calculations. The results indicate that the superior neutron shielding potential of magnetite concrete over ordinary concrete is maintained within realistic ranges of material variability.
6. The presented elemental compositions and hydrogen determination methodology provide a reliable basis for future neutronic modelling and shielding design for IFMIF-DONES and other fusion-related facilities.

CRediT authorship contribution statement

Tomasz Piotrowski: Writing – review & editing, Supervision, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Maja Kepniak:** Writing – original draft, Visualization, Formal analysis, Data curation, Conceptualization. **Elżbieta Horszczaruk:** Methodology, Investigation, Data curation,

Conceptualization. **Maria Jose Martinez-Echevarria:** Writing – original draft, Data curation, Conceptualization. **Rafał Michalczyk:** Writing – review & editing, Investigation, Data curation. **Armando Arvizu-Montes:** Writing – original draft, Visualization, Data curation. **Łukasz Ciupiński:** Writing – original draft, Formal analysis. **Santiago Becerril Jarque:** Supervision, Funding acquisition, Conceptualization. **Kazimierz Józefiak:** Writing – review & editing, Visualization. **Yuefeng Qiu:** Writing – review & editing, Investigation, Formal analysis, Conceptualization. **Martin Ansoorge:** Writing – original draft, Validation. **Hari Chohan:** Writing – review & editing, Resources, Formal analysis, Data curation. **Magdalena Grodkowska:** Visualization, Data curation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No. 101052200 – EUROfusion).

Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Data availability

Data will be made available on request.

References

- [1] W. Królas, The IFMIF-DONES fusion oriented neutron source: evolution of the design, *Nucl. Fusion*. 61 (12) (2021) 125002, <https://doi.org/10.1088/1741-4326/ac318f>.
- [2] A. Ibarra, The European approach to the fusion-like neutron source: the IFMIF-DONES project, *Nucl. Fusion*. 59 (6) (2019) 65002, <https://doi.org/10.1088/1741-4326/ab0d57>.
- [3] Y. Qiu, Overview of recent advancements in IFMIF-DONES neutronics activities, *Fusion. Eng. Des.* 201 (4) (2024) 114242, <https://doi.org/10.1016/j.fusengdes.2024.114242>.
- [4] T. Piotrowski, Optimization and evaluation of structural and shielding concrete for IFMIF-DONES, *Nucl. Mater. Energy* 38 (3) (2024) 101597, <https://doi.org/10.1016/j.nme.2024.101597>.
- [5] S.A. Thibeault, J.H. Kang, G. Sauti, C. Park, C.C. Fay, G.C. King, Nanomaterials for radiation shielding, *MRS Bull.* 40 (10) (2015) 836–841, <https://doi.org/10.1557/mrs.2015.225>.
- [6] A. Gohel, R. Makwana, B. Soni, Evaluating Shielding Materials for High Energy Space Radiation, *IOP Conf. Ser. Mater. Sci. Eng.* 1221 (1) (Mar. 2022) 12003, <https://doi.org/10.1088/1757-899X/1221/1/012003>.
- [7] S.M. Malkapur, H. Satdive, M.C. Narasimhan, N.B. Karkera, P. Goverdhan, V. Sathian, Effect of mix parameters and hydrogen loading on neutron radiation shielding characteristics of latex modified concrete mixes, *Prog. Nucl. Energy* 83 (2015) 8–12, <https://doi.org/10.1016/j.pnucene.2015.02.010>.
- [8] D.M. Nguyen, et al., Synergistic influences of stearic acid coating and recycled PET microfibers on the enhanced properties of composite materials, *Materials* 13 (6) (2020), <https://doi.org/10.3390/ma13061461>.
- [9] S. Thibeault, et al., Radiation shielding materials containing hydrogen, boron, and nitrogen: systematic computational and experimental study-phase I. NIAC Final Report, 2012.
- [10] C.V. More, Z. Alsayed, M.S. Badawi, A.A. Thabet, P.P. Pawar, Polymeric composite materials for radiation shielding: a review, *Environ. Chem. Lett.* 19 (3) (2021) 2057–2090, <https://doi.org/10.1007/s10311-021-01189-9>.
- [11] K. Shahzad, et al., Views on radiation shielding efficiency of polymeric composites/nanocomposites and multi-layered materials: current state and advancements, *Radiation* 3 (1) (2023) 1–20, <https://doi.org/10.3390/radiation3010001>.
- [12] M. Özcan, C. Kaya, F. Kaya, Cosmic radiation shielding property of boron reinforced continuous fiber nanocomposites produced by electrospinning, *Discov. Nano* 18 (1) (2023) 152, <https://doi.org/10.1186/s11671-023-03940-3>.

- [13] A. Gohel, R. Makwana, Multi-layered shielding materials for high energy space radiation, *Radiat. Phys. Chem.* 197 (2022) 110131, <https://doi.org/10.1016/j.radphyschem.2022.110131>.
- [14] C. Avcioglu, M.F. Bekheet, R. Artir, Radiation shielding and mechanical properties of mullite-zirconia composites fabricated from investment-casting shell waste, *J. Mater. Res. Technol.* 24 (2023) 5883–5895, <https://doi.org/10.1016/j.jmrt.2023.04.190>.
- [15] D. Shi, et al., Evaluation of technical and gamma radiation shielding properties of sustainable ultra-high performance geopolymer concrete, *Constr. Build. Mater.* 436 (2024) 137003, <https://doi.org/10.1016/j.conbuildmat.2024.137003>.
- [16] L. Han, et al., Constructing polymetallic nanohybrids from waste for unrivaled fluoride and phosphorus capture, *Sustain. Mater. Technol.* 44 (2025) e01418, <https://doi.org/10.1016/j.susmat.2025.e01418>.
- [17] J. Wood, *Computational Methods in Reactor Shielding*, Pergamon Press, New York, 1982.
- [18] A.B. Chilton, J.K. Shultis, R.E. Faw, *Principles of Radiation Shielding*, Prentice Hall, Englewood Cliffs, New Jersey, 1984.
- [19] M.F. Kaplan, *Concrete Radiation Shielding*, John Wiley & Sons, New York, 1989.
- [20] A.E. Profio, *Radiation Shielding and Dosimetry*, John Wiley & Sons, New York, 1979.
- [21] A.M. El-Khayatt, Calculation of fast neutron removal cross-sections for some compounds and materials, *Ann. Nucl. Energy* 37 (2) (2010) 218–222, <https://doi.org/10.1016/j.anucene.2009.10.022>.
- [22] A.M. El-Khayatt, A. El-Sayed Abdo, MERCSE-N: A program for the calculation of fast neutron removal cross sections in composite shields, *Ann. Nucl. Energy* 36 (6) (2009) 832–836, <https://doi.org/10.1016/j.anucene.2009.01.013>.
- [23] K.S. Mann, Toolkit for fast neutron removal cross-section. International Conference on Advanced Engineering and Technology (ICAET 2015), Aug. 2015 [Online]. Available: https://www.researchgate.net/profile/Kulwinder_Mann/publication/328927463_Use_WinNC-Toolkit/data/5bebc64b4585150b2bb4f236/WinNC-Toolkit.pdf.
- [24] Y. Elmahroug, B. Tellili, C. Souga, K. Manai, ParShield: a computer program for calculating attenuation parameters of the gamma rays and the fast neutrons, *Ann. Nucl. Energy* 76 (2) (2015) 94–99, <https://doi.org/10.1016/j.anucene.2014.09.044>.
- [25] S. Glasstone, A. Sesonske, *Nuclear Reactor Engineering*, third ed., CBS Publishers & Distributors, Shahdara, Delhi, 1986.
- [26] T. Piotrowski, Neutron shielding evaluation of concretes and mortars: a review, *Constr. Build. Mater.* 277 (2021) 122238, <https://doi.org/10.1016/j.conbuildmat.2020.122238>.
- [27] V.F. Sears, Neutron scattering lengths and cross sections of the elements and their isotopes, *Neutron. N.* 3 (3) (1992) 29–37.
- [28] N. C. for N. Research, “Neutron scattering lengths and cross sections database.” Aug. 2024. [Online]. Available: <https://www.ncnr.nist.gov/resources/n-lengths/>.
- [29] P. Prochon, T. Piotrowski, The effect of cement and aggregate type and w/c ratio on the bound water content and neutron shielding efficiency of concretes, *Constr. Build. Mater.* 264 (2020) 120210, <https://doi.org/10.1016/j.conbuildmat.2020.120210>.
- [30] K. Zalegowski, Relation between microstructure, technical properties and neutron radiation shielding efficiency of concrete, *Constr. Build. Mater.* 235 (2020) 117389, <https://doi.org/10.1016/j.conbuildmat.2019.117389>.
- [31] M.A. Masoud, Valorization of hazardous chrysotile by H3BO3 incorporation to produce an innovative eco-friendly radiation shielding concrete: implications on physico-mechanical, hydration, microstructural, and shielding properties, *Cem. Concr. Compos.* 141 (2023) 105120, <https://doi.org/10.1016/j.cemconcomp.2023.105120>.
- [32] T. Piotrowski, M. Mazgaj, A. Żak, J. Skubalski, Importance of atomic composition and moisture content of cement-based composites in neutron radiation shielding, *Procedia Eng.* 108 (2015) 616–623, <https://doi.org/10.1016/j.proeng.2015.06.188>.