



Comprehensive Evaluation of Materials for Fusion Reactor Applications: A PACBDHTE Approach

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Abstract: This study introduces a new framework, PACBDHTE, designed to evaluate materials for fusion reactor applications. To provide an integrated assessment that encompasses radiation damage, hydrogen behavior, transmutation effects, and material erosion within a unified evaluation scheme. The methodology includes evaluation Displacement per Atom (DPA) calculations, hydrogen retention analysis, transmutation assessments, and erosion rate determinations. The results identified SiC and WC-Be are strong candidates due to their exceptional hydrogen retention capabilities. Tungsten-based materials are competitive, but careful consideration is needed for 316L stainless steel due to lower hydrogen retention. additionally, Cu(I)-functionalized metal-organic frameworks (MOFs), such as Cu(I)-MFU-4l, show promising selectivity for hydrogen isotope separation which can support more efficient fusion fuel-cycle management. Overall, the findings highlight erosion rates are critical for material longevity, emphasizing the need for continuous monitoring. Overall, the study contributes to safe and efficient fusion energy technology.

Keywords: Tungsten based alloys; Metal-organic frameworks; Monte Carlo simulations; High energy neutrons; Nuclear fusion energy; Clean and sustainable power source; Controlled fusion reactions

1 Introduction

The pursuit of nuclear fusion energy as a clean and sustainable power source holds fascinating promise in meeting the burgeoning energy demands of our world [1] while concurrently mitigating the environmental impact of conventional energy generation [2]. However, the journey to harnessing fusion energy's potential is fraught with formidable challenges, chief among them being the creation and maintenance of extreme conditions that facilitate controlled fusion reactions [3]. The lofty temperatures and pressures within fusion reactors can subject materials to degradation, while the generation of high-energy neutrons presents risks of equipment damage and radioactive waste [4].

Among the many complexities of fusion energy development, the selection of structural materials stands as an important factor in ensuring the viability and success of controlled nuclear fusion [5]. Particularly, the choice of Plasma Facing Material (PFM) emerges as a pivotal decision, given its direct exposure to the plasma environment and its important role in containing the fusion reactions while enduring extreme heat and radiation [6, 7].

Amidst the search for optimal PFMs, tungsten has emerged as a leading contender due to its exceptional mechanical properties and remarkable resistance to radiation [8, 9]. Nevertheless, previous studies have not fully addressed its high melting point, thermal conductivity and resilience to erosion make it an attractive candidate for the challenging fusion environment. However, the way to realizing tungsten's potential is not without its complexities [10]. The interaction with fusion neutrons leads to a transmutation phenomenon that transforms tungsten into osmium, through rhenium, which presents a significant concern within the context of a fusion power plant. Moreover, the primary damage induced by radiation can lead to alterations in tungsten's microstructure, influencing its thermal and mechanical characteristics [11, 12].

Table 1. Comparative summary of key materials for nuclear fusion applications

Material/System	Function in Fusion	Key Properties	Advantages	Limitations
Tungsten (W)	Plasma-facing material (PFM)	High melting point, thermal conductivity, sputter resistance	Excellent thermal stability and erosion resistance	Neutron transmutation ($W \rightarrow Re \rightarrow Os$), radiation-induced brittleness [13–16]
WC–Be	PFM candidate	Composite of tungsten carbide and beryllium	High thermal resistance and low atomic number (Be)	Toxicity of Be, complex mechanical behavior under irradiation [17, 18]
W–Fe–Mo	PFM candidate	Alloy of W with Fe and Mo	Tunable mechanical and thermal properties	Radiation-induced phase instability [17]
316L Stainless Steel	Structural/fuel component	Austenitic stainless steel, moderate radiation resistance	Readily available, great corrosion resistance	Poor resistance to high neutron flux and swelling [18]
SiC (Silicon Carbide)	PFM/Structural material	Ceramic with high thermal stability and low neutron absorption	Radiation resistance, low activation	Brittle nature, fabrication complexity [17, 18]
Cu(I)-MOFs	Isotope separation (peripheral systems)	Porous crystalline materials with Cu(I) active sites	High selectivity for D_2/T_2 over H_2 , low-temperature operation	Not thermally stable enough for core plasma exposure [19, 20]
Cu(I)-MFU-4l	Isotope separation in fuel cycle (D_2 , T_2)	High selectivity for D_2 over H_2 (~ 11 at 100 K); Cu(I)-functionalized	Allows tritium purification; β -radiation resistance	Thermally unstable at fusion-relevant core temperatures [19]
W–Ta–Cr–V/WxTaTiVCr	High-Entropy Alloys (HEAs) as PFM candidates	Multi-principal element alloys	Excellent radiation damage resistance and thermal performance	Limited experimental data in fusion conditions [13, 21]

To address these intricate challenges, a comprehensive study of the radiation behavior of plasma-facing materials within the fusion environment turns indispensable [22]. This article focuses on tungsten-based alloys as potential candidates for plasma-facing applications and aim to unravel the effects of neutron radiation on these materials [23]. Through advanced Monte Carlo simulations, the radiation damage inflicted on various candidate materials, including WC-Be, W-Fe-Mo, SiC, and 316L SS, is meticulously assessed [17, 18]. The ultimate objective is to identify a PFM that excels in two vital aspects: transmutation behavior and radiation damage resistance [24].

Furthermore, metal-organic frameworks (MOFs) have recently emerged as promising materials for the separation and containing of hydrogen isotopes—particularly deuterium and tritium—which are critical in nuclear fusion fuel cycles. a Cu(I)-functionalized MOF known as Cu(I)-MFU-4l demonstrated exceptional selectivity for deuterium over hydrogen D_2 -over- H_2 selectivity of approximately 11 at 100 K, indicating strong potential for tritium capture and purification [19]. More recent studies identified Cu(I)-MOF as having enhanced β -radiation resistance and the capability to operate at higher temperatures [20]. Although MOFs are not as good as direct plasma-facing materials (PFMs) due to thermal limitations, they hold promise in peripheral systems for isotope management or as precursors for advanced ceramic PFMs via MOF-derived synthesis strategies. These findings highlight MOFs’ potential role in enhancing the sustainability of fusion fuel cycles through selective isotope control and material innovation.

The International Thermonuclear Experimental Reactor (ITER) project represents a significant milestone in nuclear fusion research [25, 26], demonstrating the feasibility of fusion as clean and abundant energy source [27]. A central challenge of ITER is selecting suitable plasma-facing materials that can withstand the hard conditions of fusion reactions [26].

This selection process involves considering factors like radiation resistance, thermal conductivity, erosion rates, and compatibility with fusion fuels. The use of Entropy Element Materials (HEMs) has gained attention, with

materials like W-Ta-Cr-V and WxTaTiVCr [28] showing potential due to their resistance to radiation damage [21]. However, the choice between body-centered cubic (BCC) and face-centered cubic (FCC) structures also plays an important role in radiation resistance.

Tungsten's suitability as a plasma-facing material is due to its magnificent physical properties, including high melting point, thermal conductivity, and sputter resistance [13–15]. Despite its advantages, the interaction of tungsten with fusion neutrons leads to transmutation, transforming the material into osmium via rhenium [13]. This transmutation phenomenon poses challenge in managing material integrity within a fusion power plant. Furthermore, radiation-induced damage changes the microstructure of tungsten, affecting its mechanical and thermal characteristics [15]. Table 1 provides a comparative summary of their key properties and potential in nuclear fusion applications.

Radiation damage evaluation involves understanding the effects of high-energy particles on materials, resulting in atomic displacement, defect creation, and differences in mechanical properties [26]. Various computational methods, such as molecular dynamics and Monte Carlo simulations, enable accurate prediction of Displacements per Atom (DPA) accumulation in materials exposed to radiation. These simulations aid in assessing the impact of radiation on materials' long-term performance [16].

A thorough understanding of radiation behavior and material response is important for advancing nuclear fusion technology [29]. In the quest for controlled nuclear fusion, researchers must navigate intricate challenges associated with radiation-induced material damage and transmutation phenomena. By addressing these complexities, the field of materials science for fusion reactors can make informed decisions to develop plasma-facing components that ensure enhanced safety, efficiency, and extended lifespan [16]. As researchers delve deeper into the complexities of radiation behavior in fusion environments, they embark on a journey that brings controlled nuclear fusion one step closer to finding the boundless potential of fusion energy for a sustainable tomorrow [30]. However, the path to reliable fusion energy is still hindered by the absence of a unified approach for evaluating materials under the hard conditions of a fusion reactor. Existing studies often separate single properties—such as radiation damage, hydrogen retention, or erosion—without fully capturing the complex interactions that dictate long-term material performance. This gap limits the development of plasma-facing components that can ensure both safety and efficiency over extended operational lifetimes.

Unlike previous research, our approach simultaneously evaluates the PACBDHTE framework, a comprehensive evaluation method that integrates DPA calculations, hydrogen retention analysis, transmutation behavior, and erosion rate assessments. By applying this framework to candidate materials such as SiC, WC-Be, tungsten-based alloys, and Cu(I)-functionalized MOFs, we aim to find materials that can withstand the intricate balance of radiation damage and fuel cycle demands, ultimately guiding the design of fusion reactors toward enhanced durability, efficiency, and sustainability.

2 Materials and Methods

In this study, we employ the newly established PACBDHTE (Performance Assessment Criteria based on DPA, Hydrogen retention, Transmutation, and Erosion rate) to comprehensively evaluate materials for potential fusion reactor applications.

2.1 Materials Selection

In the current study, we selected candidate materials for potential fusion reactor applications. The materials evaluated include WC-Mo-Fe, WC-Be, WC-Ti, 316L Stainless Steel, WC-Ti-B-Fe, W-Ti-B-Fe, and SiC. These materials were chosen based on their properties, such as high-temperature stability, mechanical strength, and resistance to radiation damage. The compositions, theoretical densities, and relevant material parameters used for PHITS and Stopping and Range of Ions in Matter (SRIM) simulations are summarized in Table 2. The theoretical densities were calculated using CALPHAD software and served as the input densities for all simulations to ensure consistency and reproducibility.

2.2 PHITS Modelling

PHITS is a versatile Monte Carlo code capable of simulating irradiation, particle transport, and analysis across a vast energy spectrum. In this study, PHITS was employed to assess radiation damage by calculating DPA and analyzing material transmutation.

2.2.1 Radiation damage model in PHITS

Radiation damage has long been an interesting subject, with DPA as the typical damage metric. PHITS incorporates an advanced approach that integrates a non-thermal composite correction model with a conventional Monte Carlo framework to calculate arc-DPA values corresponding to DDDeff [18]. Kinchin and Pease established

the foundation for an early model to estimate DPA by accounting for kinetic energy transfers exceeding a material-specific threshold displacement energy. In this model, the predicted number of atomic displacements (N_d) is expressed as a function of cascade energy, also known as the damage function [31].

Table 2. The theoretical densities of the selected materials

Material No.	Element	wt%	Theoretical Density
1	W	90	15.51096
	Mo	5	0.88128
	Fe	5	0.881888
	Total		17.274128
2	W	95.25	17.15958
	C	0.38	0.06842
	Mo	3.03	0.5457
	Fe	1.25	0.2251964
	Total		17.9988964
3	W	90	9.235755
	C	5	0.52492
	Be	5	0.5250168
	Total		10.2856918
4	W	90.96	11.317075
	C	5.93	0.737664
	Ti	3.1	0.38565
	Total		12.440389
5	W	18.9	1.104885
	C	1.02	0.05808
	Ti	20	1.1691
	B	20	1.16909
	Fe	20	1.169289
	Total		4.670444
6	W	25	1.19583
	Ti	25	1.19655
	B	25	1.19669
	Fe	25	1.196848
	Total		4.785918
7	Si	70.0044	1.61702
	C	29.99552	0.69156
	Total		2.30858
8 (316L)	Fe	61.8	4.842642519
	Cr	17	1.332118478
	Ni	13.5	1.057858761
	Mo	2.5	0.195899792
	Mn	1.5	0.117539871
	Si	1	0.078359904
	C	0.03	0.002350807
	P	0.05	0.003917987
	S	0.03	0.002350796
	N	0.1	0.007835993
	Totals	100	7.640874908

$$N_d(T_d) = \begin{cases} 0, & T_d < E_d \\ 1, & E_d < T_d < \frac{2E_d}{0.8} \\ \frac{0.8T_d}{2E_d}, & \frac{2E_d}{0.8} < T_d < \infty \end{cases} \quad (1)$$

where, T_d represents the damage energy, which is the kinetic energy available for generating atomic displacements. E_d denotes the threshold displacement energy, defined as the minimum energy required for an atom to be displaced from its lattice position. energy minus the energy lost to electronic interactions (ionization). This is essentially the

Kinchin–Pease model, except that the original kinetic energy term was replaced by the damage energy to account for ionization effects and a factor of 0.8 was found to account for more realistic interatomic potentials.

Building upon Nordlund’s earlier work [32], the non-thermal composite corrected-per-atom displacement (arc-DPA) is outlined in detail by Nordlund et al. [33].

$$N_{d,atrua}(T_d) = \begin{cases} 0, T_d < E_d \\ 1, E_d < T_d < \frac{2E_d}{0.8} \\ \frac{0.8T_d}{2E_d} G_{adpa}, \frac{2E_d}{0.8} < T_d < \infty \end{cases} \quad (2)$$

with the new efficiency function $\xi_{arcDPA}(T_d)$ given by Mohammed [4].

$$\zeta_{arcDPA}(T_d) = \frac{1 - \zeta_{arcDPA}}{\left(\frac{2E_d}{0.8}\right)^{barredpa}} T_d^{barcupa} + C_{arcDPA} \quad (3)$$

In this context, E_d represents the average threshold displacement energy, consistent with the value used in the NRT-DPA model. Additionally, $barredpa$ and C_{arcDPA} are material-specific constants that must be determined through molecular dynamics (MD) simulations or experimental measurement.

2.3 Transmutation Modeling in PHITS

In Transmutation simulation is carried out for the selected four materials using PHITS. For transmutation calculation, DCHAIN is used to calculate the time variation of induced activities, decay heats, γ -ray spectra and dose rates. It is a decay, burnup and activation code. It is made to track production and destruction of nuclide inventories as a function of time over any time scale. The general process of the flow is visualized as shown in Figure 1.

Firstly, the target geometry is built as shown in Figure 2. A beam of 10 MeV neutrons is incident on a rectangular-prism-shaped target composed of three segments: tungsten, water, and iron. The scope of this project is focused on the first layer of the box where it is treated as plasma facing material for the fusion reactor. The first layer will This box is surrounded by beryllium on the sides and back. This structure is irradiated with a beam current of 100 nA for 10 minutes and then left to cool for 50 minutes total.

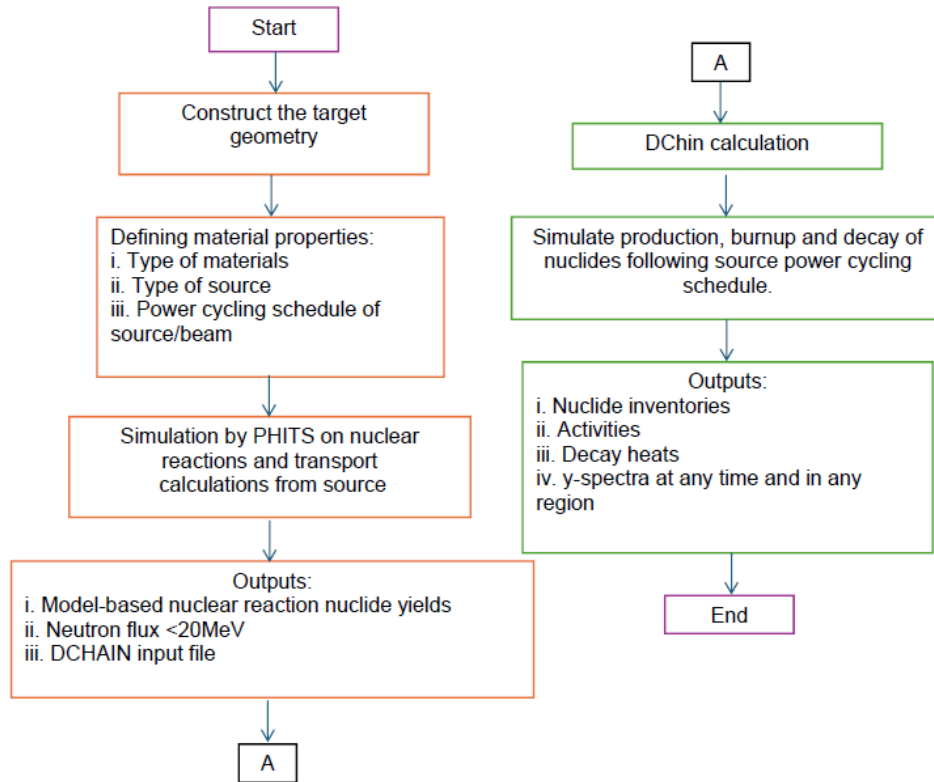


Figure 1. Process flow chart of DChain module

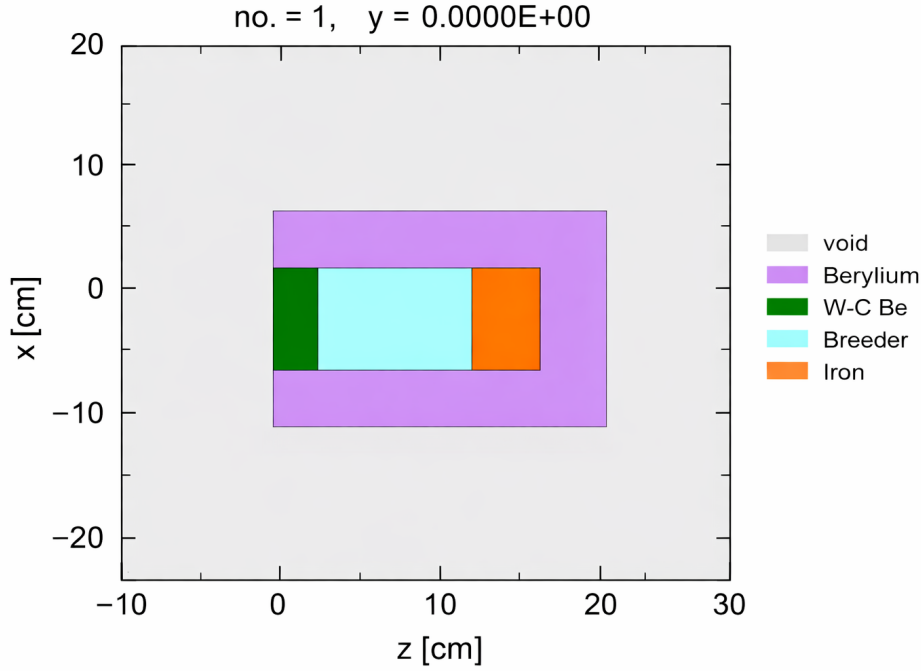


Figure 2. Target geometry

PHITS Next, PHITS automatically generates an input file for DCHAIN by using the [t-dchain] tally. Then, the calculation is carried out using DCHAIN to get the output file containing information on the radioactive activities, dose rates, decay heats and more. Table 3 illustrate the parameter that is used for the code is as follows:

- (i) The number of neutron bombardment is 2000.
- (ii) The energy of neutron radiation is 10MeV.
- (iii) The materials that are used for the first layer are WC-Be, W-Fe-Mo, SiC and 316L ss.
- (iv) Calculation data is as below:

Table 3. Calculation data used in PHITS

Parameter	Value
Beam current	0.0001 mA
Beam energy	3 GeV
Beam power	0.0003 MW
Neutron flux	$1.7007 \times 10^{10} \text{ n} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$
Region volume	192 cm^3
Irradiation time	2 h

2.4 Stopping and Range of Ions in Matter Module

The SRIM is a widely used simulation tool made to evaluate ion interactions with materials. It provides insights into ion implantation, sputtering, and damage effects, making it particularly useful for studying hydrogen retention and erosion rates in fusion reactor materials. SRIM works by modeling ion trajectories based on energy loss mechanisms, including nuclear and electronic stopping processes, enabling precise calculations of material responses under ion bombardment.

2.4.1 Hydrogen retention analysis

SRIM is employed to simulate hydrogen ion implantation and track penetration depth, energy dissipation, and retention behavior within the selected materials. By analyzing ion distribution profiles, it helps quantify hydrogen accumulation and predict retention capacity, which is vital for assessing material performance in plasma-facing environments.

2.4.2 Erosion rate evaluation

The erosion rate of a material due to plasma exposure can be calculated using a simplified formula as following:

$$E = F \times Y \quad (4)$$

where,

E = Erosion rate (e.g., in $\text{\AA}^2/\text{s}$)

F = Incident ion flux (ions/ $\text{\AA}^2/\text{s}$)

Y = Sputtering yield (dimensionless or unitless, representing the ratio of sputtered atoms/collided ion)

Also, it is seen that studying neutron irradiation in SRIM can be used by the ideal representation of monoatomic hydrogen, which by nature has approximately similar atomic mass of 1 amu as that of a neutron.

3 Results

3.1 Displacement per Atom (DPA)

The assessment of DPA serves as a critical indicator of radiation-induced damage potential in materials intended for fusion reactor applications.

The calculated DPA values for the candidate materials under neutron radiation at 10 MeV are integral to the evaluation of their suitability in these environments. Among the materials studied, as observed from Figure 3, W-Mo-Fe demonstrates notably low DPA values, indicating a high degree of resistance to radiation-induced displacement of atoms. This characteristic positions it as a great candidate for components exposed to neutron irradiation. Conversely, 316L stainless steel exhibits significantly higher DPA values, signalling greater susceptibility to radiation damage. While 316L boasts multiple desirable properties, its radiation resistance may necessitate additional considerations or protective measures in specific reactor application.

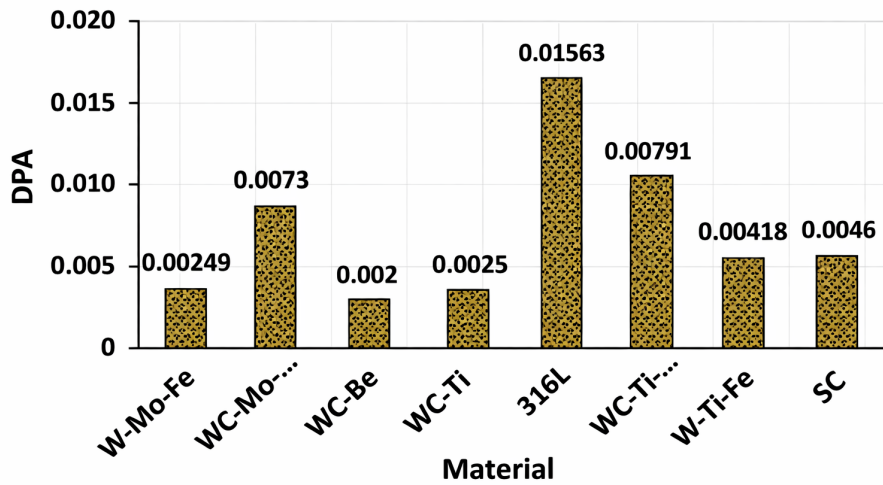


Figure 3. Displacement per Atom (DPA) of the candidate materials

Suggesting their potential suitability for fusion reactor components subjected to neutron irradiation. The choice of materials for these critical applications should involve a balanced consideration of various factors, including DPA results, thermal, mechanical, and corrosion resistance, and the expected neutron flux in each operational context. These DPA finding thus provide valuable insights into the radiation resilience of candidate materials, guiding informed material selection for fusion reactor components.

3.2 Nuclear Transmutation

The presented data encompasses a comprehensive assessment of transmutation effects and radiological parameters for materials intended for fusion reactor applications. This analysis holds a great importance in ensuring the safety of both personnel and the environment in the context of fusion energy production. Notably, the materials WC-Ti and W-Mo-Fe show distinct transmutation profiles as presented in Table 4 and Table 5.

Table 4. Results of the radioactivity for each material

Material	Nuclide	Atoms (atoms/cm ³)	Radioactivity (Bq/cm ³)	Total Radioactivity (Bq)	Relative Error
WC-Ti	Sc-48	1.26×10^9	5.54×10^3	1.06×10^6	8.81×10^{-3}
W-Mo-Fe	Lu-176	2.21×10^{-2}	1.29×10^{-20}	8.26×10^{-19}	2.88×10^{-2}
SiC	Mg-28	1.26×10^{-4}	1.16×10^{-9}	7.40×10^{-8}	7.12×10^{-2}
316L	V-50	1.80×10^{10}	2.84×10^{-15}	1.82×10^{-13}	6.24×10^{-3}
	Nb-91	4.05×10^7	1.34×10^{-3}	2.57×10^{-1}	7.97×10^{-3}
	Nb-92	1.04×10^9	6.56×10^{-7}	1.26×10^{-4}	7.97×10^{-3}
WC-Mo-Fe	Nb-94	2.39×10^8	2.59×10^{-4}	4.97×10^{-2}	1.34×10^{-2}
	Mo-93	6.36×10^8	3.39×10^{-3}	6.51×10^{-1}	9.22×10^{-3}
	Tc-98	2.61×10^{-4}	1.36×10^{-18}	2.61×10^{-16}	2.49×10^{-2}
	Hf-182	5.73×10^3	1.08	2.07×10^2	7.05×10^{-3}
	Lu-177m	1.38×10^{-10}	6.88×10^{-18}	1.32×10^{-15}	3.30×10^{-2}
WC-Be	Hf-182	1.01×10^5	2.49×10^{-10}	4.77×10^{-8}	7.48×10^{-3}
	Ta-179	6.82×10^8	8.24	1.58×10^3	1.08×10^{-2}
	Ca-45	9.42×10^9	4.65×10^2	8.92×10^4	8.28×10^{-3}
W-Ti-B-Fe	Mn-54	3.93×10^{10}	1.01×10^3	1.94×10^5	7.09×10^{-3}
	Fe-55	9.00×10^8	7.20	1.38×10^3	7.09×10^{-3}
	Co-60	5.82×10^{-4}	2.42×10^{-12}	4.65×10^{-10}	7.57×10^{-2}
	Ca-45	9.35×10^9	4.61×10^2	8.86×10^4	8.13×10^{-3}
WC-Ti-B-Fe	Mn-54	3.94×10^{10}	1.01×10^3	1.94×10^5	7.14×10^{-3}
	Fe-55	9.14×10^8	7.32	1.40×10^3	7.14×10^{-3}
	Co-60	1.60×10^{-3}	6.65×10^{-12}	1.28×10^{-9}	8.99×10^{-2}

Table 5. Results of decay rate, half-life and dose rate for each material

Material	Decay heat		Total	Half-Life (s)	Dose-Rate (uSv·m ² /h)
	Beta	Gamma			
WC-Ti	1.96E-10	2.98E-09	3.17E-09	1.57E+0	5.62E+0
W-Mo-Fe	6.14E-34	9.92E-34	1.61E-33	1.19E+18	6.86E-25
SiC	2.98E-23	2.54E-22	2.84E-22	7.53E+04	1.62E-13
316L	7.14E-30	6.46E-28	6.53E-28	4.40E+24	3.82E-19
	1.10E-18	2.23E-18	3.33E-18	2.10E+10	7.01E-09
	7.58E-22	1.59E-19	1.60E-19	1.10E+15	3.17E-10
WC-Mo-Fe	6.14E-18	6.53E-17	7.15E-17	6.40E+11	1.32E-07
	2.72E-18	5.87E-18	8.58E-18	1.30E+11	1.95E-08
	2.57E-32	3.07E-31	3.33E-31	1.33E+14	6.31E-22
	2.58E-24	9.54E-24	1.21E-23	2.81E+14	1.99E-14
	8.73E-32	1.85E-31	2.72E-31	1.39E+07	3.74E-22
WC-Be	2.57E-24	9.48E-24	1.21E-23	2.81E+14	1.97E-14
	6.03E-15	3.52E-14	4.12E-14	5.74E+07	1.65E-04
	5.72E-12	8.89E-19	5.72E-12	1.41E+07	1.09E-10
W-Ti-B-Fe	6.45E-13	1.35E-10	1.36E-10	2.70E+07	2.70E-01
	4.58E-15	1.96E-15	6.55E-15	8.66E+07	4.04E-13
	3.76E-26	9.73E-25	1.01E-24	1.66E+08	1.79E-15
	5.68E-12	8.83E-19	5.68E-12	1.41E+07	1.08E-10
WC-Ti-B-Fe	6.46E-13	1.36E-10	1.36E-10	2.70E+07	2.71E-01
	4.65E-15	2.00E-15	6.65E-15	8.66E+07	4.10E-13
	1.03E-25	2.67E-24	2.77E-24	1.66E+08	4.91E-15

WC-Ti, featuring Sc48, exhibits increased radioactivity and decay heat production, resulting in a notable dose rate of 5.62 uSv·m²/h, underlining its radiological impact. In contrast, W-Mo-Fe, characterized by Lu176, shows minimal radioactivity and decay heat production, leading to an exceptionally low dose rate of 6.86E-25 uSv·m²/h, indicating a negligible radiological impact. SiC shows transmutation effects with Mg28, leading to moderate radioactivity and decay heat production, resulting in a dose rate of 1.62E-13 uSv·m²/h, which should be considered in safety assessments.

As showed in Table 5 in the case of 316L, V50 contributes to an increased radioactivity and decay heat, yielding

a dose rate of $3.82\text{E-}19$ uSvm²/h, emphasizing the importance of radiological safety considerations for this material. Moving on to materials like WC-Mo-Fe and WC-Be, they exhibit complex transmutation profiles with multiple nuclides, resulting in varying level of radioactivity and decay heat production. Dose rates range from $7.01\text{E-}09$ to $3.17\text{E-}10$ uSvm²/h, underscoring the need for comprehensive radiological assessments to ensure safety in fusion reactor applications.

Notably, Ta179 stands out due to its magnificent radioactivity and decay heat production, resulting in a substantial dose rate of $1.65\text{E-}04$ uSvm²/h. This nuclide demands meticulous consideration concerning radiological safety. Within W-Ti-B-Fe, various nuclides exhibit diverse levels of radioactivity and decay heat production, leading to dose rates ranging from $1.09\text{E-}10$ to $2.70\text{E-}01$ uSvm²/h, highlighting the great need for thorough radiological assessments. Finally, WC-Ti-B-Fe showcases transmutation effects with diverse dose rates ranging from $1.08\text{E-}10$ to $2.71\text{E-}01$ uSvm²/h, emphasizing the diverse radiological profiles of these materials and their importance in material selection and reactor design for safe fusion energy production. reactor. Similarly, materials like W-Ti-B-Fe and WC-Mo-Fe display erosion rates of 20 A²/s, indicating substantial erosion effects. This information underscores the importance of continuous monitoring and maintenance when these materials are employed.

3.3 Hydrogen (H) Retention

The assessment of hydrogen retention is a pivotal aspect of material selection for fusion reactor applications. At 10 keV ion energy, the materials under investigation shows varying levels of hydrogen retention, which significantly impact their suitability for plasma-facing components in fusion reactors.

SiC emerges as a standout performer, exhibiting the highest hydrogen retention depth of 678.06 μm . This exceptional retention capability positions SiC as an excellent choice for fusion reactor applications, particularly in regions exposed to high-energy ion bombardment. Its stability in retaining hydrogen ions at this energy level underscores its resilience in challenging fusion reactor environments.

WC-Be, a material known for its compatibility with fusion reactor conditions, also demonstrates robust hydrogen retention, with depth of 279.79 μm at 10 keV ion energy. This finding reaffirms the reliability of WC-Be in retaining hydrogen ions, reinforcing its role as a suitable candidate for plasma-facing components. As observed from Figure 4, Tungsten-based materials, including W-Mo-Fe, WC-Mo-Fe, WC-Ti, and WC-Ti-B-Fe, exhibit intermediate levels of hydrogen retention, with depths of penetration ranging from 176.76 μm to 240.18 μm . While these materials show competitive hydro-gen retention characteristics, their application in fusion reactors should be evaluated considering additional factors such as thermal and mechanical properties.

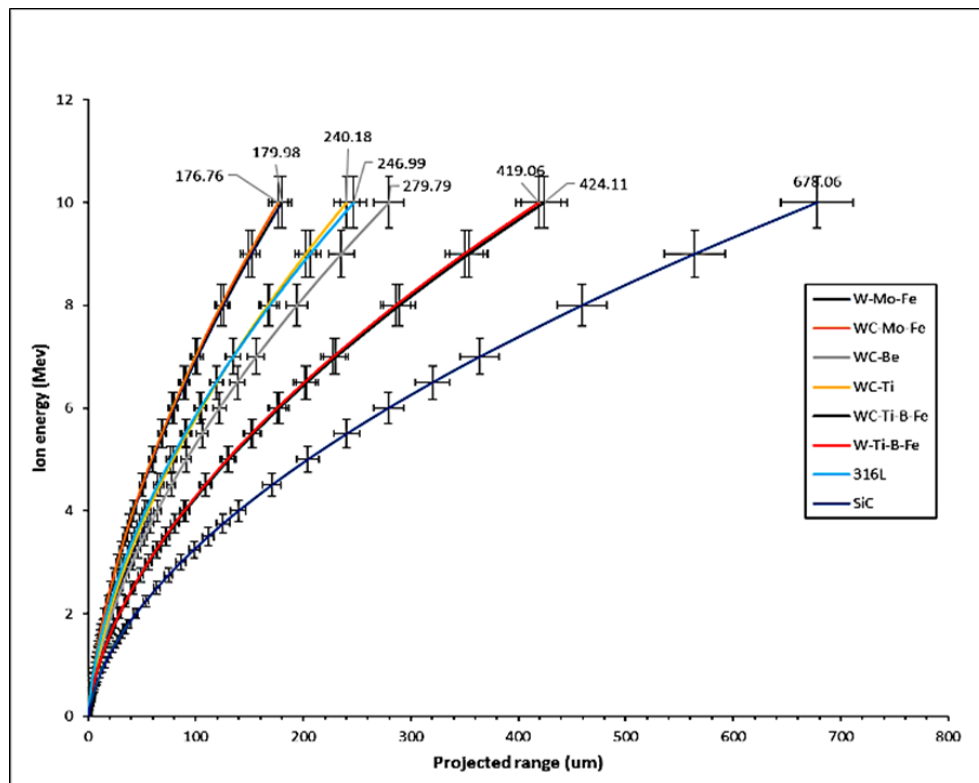


Figure 4. Hydrogen retention of the candidate materials

Conversely, 316 L stainless steel demonstrates relatively lower hydrogen retention, with a depth of 246.99 μm at 10 keV ion energy. This result considers that 316 L may be less suited for plasma-facing components, especially in scenarios involving high-energy ion bombardment, where robust hydrogen retention is imperative.

In conclusion, the maximum hydrogen retention values at 10 keV ion energy offer vital insights into the materials' performance under extreme conditions. SiC and WC-Be emerge as strong contenders, given their excellent hydrogen retention capabilities. Tungsten-based materials occupy an intermediate position, warranting consideration in specific fusion reactor applications. However, 316L stainless steel's comparatively lower hydrogen retention emphasizes the importance of judicious material selection and design considerations when implementing it in fusion reactor components exposed to high-energy ion environments. These findings help significantly to the comprehensive evaluation of materials for fusion reactor applications, ensuring the safety and efficiency of future fusion energy systems.

3.4 Erosion Rate

Atomic the transmutation and radiological characteristics discussed earlier (as shown in Figure 4), it is vital to consider the erosion rates of materials intended for fusion reactor applications, as these rates directly impact their longevity and structural integrity in a high-energy fusion environment. Among the materials examined, 316 L exhibits the highest erosion rate at 35 A^2/s , which implies a significant level of material loss over time. This necessitates careful consideration when selecting 316 L for specific components within the system.

Conversely, materials such as WC-Ti and SiC exhibit comparatively lower erosion rates at 11 A^2/s and 2 A^2/s , respectively. While these materials could experience erosion to a lesser degree, their transmutation and radiological characteristics, as discussed previously (see Figure 5), must still be carefully evaluated to ensure overall safety and performance within a fusion reactor. Of particular interest are WC-Ti-B-Fe and WC-Be, which both present erosion rates of 9 A^2/s (as depicted in Figure 5). These erosion rates, coupled with their transmutation profiles and radiological characteristics, make them interesting candidates for further investigation, as they may strike a balance between erosion resistance and radiological safety.

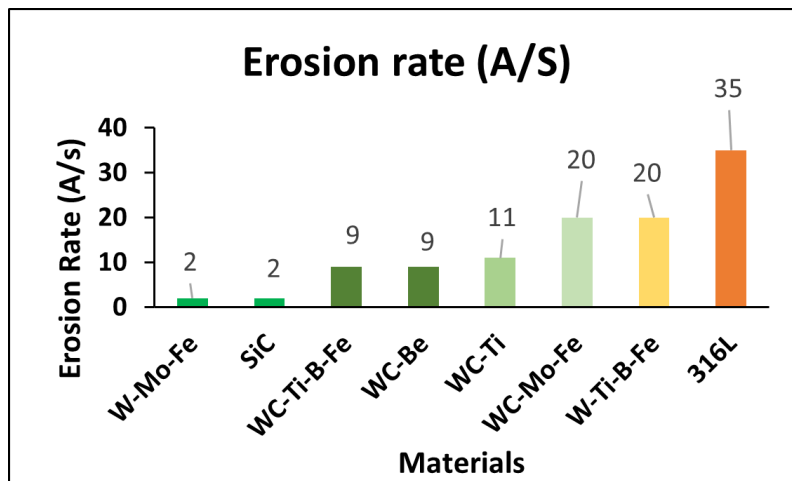


Figure 5. Erosion rate for each material under

In summary, the erosion rates of materials play an important role in their suitability for fusion reactor applications. By considering erosion rates alongside transmutation and radiological data (as presented in Figure 5), engineers and researchers can make in-formed decisions about material selection and reactor design, ultimately contributing to the safe and efficient development of fusion energy technology.

4 Discussion

A comprehensive assessment of radiation-dependent emission degradation (DPA), hydrogen retention, nuclear transmutation, and erosion rates helps to gain a deeper understanding of material performance under fusion reactor conditions. W-Mo-Fe alloys exhibit low DPA and minimal radioactive impact, making them promising structural materials. SiC and WC-Be alloys demonstrate excellent hydrogen retention and low erosion rates, indicating their suitability for plasma-facing components. Tungsten-based alloys offer moderate performance, striking a balance between hydrogen retention and acceptable radiation resistance, while 316 L stainless steel exhibits high DPA, low hydrogen retention, and a high erosion rate, suggesting the need for careful consideration or protective measures. In conclusion, material selection must strike a balance between radiation resistance, hydrogen retention, transmutation behavior, and erosion resistance to ensure the safe and efficient operation of fusion reactors.

5 Conclusions

In this study, we applied the PACBDHTE framework to evaluate materials for fusion reactor applications, considering DPA, hydrogen retention, transmutation, and erosion rates. Our results show that SiC and WC-Be are strong candidates for plasma-facing components due to their high hydrogen retention and favorable erosion resistance, while tungsten-based materials offer a balance of structural stability and radiological safety. 316 L stainless steel exhibits lower hydrogen retention, indicating the need for careful design in high-energy ion environments.

Based on these findings, W-Mo-Fe alloys are recommended for structural components due to low DPA and minimal radioactive impact, whereas SiC and WC-Be are ideal for plasma-facing applications. Looking forward, experimental validation of DPA constants (e.g., $\bar{\sigma}_{\text{dpa}}$ and $\bar{\sigma}_{\text{dpa}}$) and hydrogen-retention behavior is recommended to further refine material selection and ensure predictive accuracy of the PACBDHTE framework. Overall, this work provides a data-driven approach for material selection and reactor design, supporting the development of safe, efficient, and sustainable fusion energy technology.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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