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Scoping of material response under DEMO neutron irradiation: Comparison with fission and influence of nuclear library selection

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HIGHLIGHTS

- Inventory calculations for all naturally occurring elements from H to Bi.
- Helium and hydrogen production is compared for different elements.
- DEMO fusion first-wall results are compared against fission.
- Calculations with different nuclear data libraries.
- He-to-dpa and H-to-dpa ratios are computed for fusion and fission.

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ABSTRACT

Predictions of material activation inventories are an important input into the operational, safety and environmental assessment of future fusion nuclear plants. Additionally, the neutron-induced transmutation (change) of material composition (inventory) with time, and the creation and evolution of configurational damage from atomic displacements, require precise quantification because they can lead to significant changes in material properties, and thus influence reactor-component lifetime. A comprehensive scoping study has been performed to quantify the activation, transmutation (depletion and build-up) and immediate damage response under neutron irradiation for all naturally occurring elements from hydrogen to bismuth. The resulting database provides a global picture of the response of a material, covering the majority of nuclear technological space, but focussing specifically on typical conditions expected for a demonstration fusion power plant (DEMO).

Results from fusion are compared against typical fission conditions for selected fusion relevant materials, demonstrating important differences and confirming that the latter cannot necessarily be relied upon to give accurate scalable experimental predictions of material response in a future fusion reactor. Results from different nuclear data libraries are also compared.

1. Introduction

Accurate predictions of material activation – as caused by nuclear reactions – are necessary because they impact the operational limits, maintenance schedule, safety and environmental impact of future fusion nuclear plants. Meanwhile, the resultant neutron-induced transmutation of material composition (inventory), including the formation of gas bubbles, and the creation and evolution of damage from atomic displacements, require precise quantification because they can lead to a change in material properties, which influence reactor-component lifetimes and hence reactor maintenance costs.

For a fully-detailed reactor design with complete materials descriptions, such as that now available for neutron-transport simulations of the ITER experimental fusion reactor currently under construction, it is entirely possible to predict the neutron irradiation at any point in the vessel. Large-scale parallel computing with modern neutron-transport codes, such as MCNP-6 [1], allow neutron spectra to be accurately predicted in the hundreds of thousands of geometric regions (cells) that describe the complex theoretical models of vessel geometries for both ITER and a future demonstration fusion power plant (DEMO). Subsequently, these predictions of neutron fields can be fed into a nuclear inventory code, such as the state-of-the-art FISPACT-II [2,3] system, to calculate the expected material activation and transmutation response

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for any reactor component at any given time during the simulated reactor operation or end-of-life (EOL) decay-cooling.

However, the design of demonstration fusion power plants (DEMOs) is still at the conceptual stage, with some of the material choices still uncertain. There is therefore scope for material selection and design studies where almost any material (element) could be considered, subject to environmental constraints. There are many factors to consider when deciding what material composition might be acceptable for a particular fusion application, including activation response. A material's compositional stability under neutron irradiation – *i.e.* how much will it transmute? –, particularly how much gases and other harmful impurities it might generate, is also an important concern, as is the associated formation of radiation damage, whose source terms (the primary knock-on atoms or PKAs) can be quantified using the nuclear interaction database [4]. These last two factors, in particular, largely determine the irradiation impact on material properties and hence the structural integrity limits (for safety) and operational life of key reactor components.

To aid the material selection decisions of nuclear engineers and scientists, and also material modellers and experimentalists, there is a need for a reference database of response measures for elements under typical fusion (and fission) conditions. Such databases have been produced before, but these are now obsolete because they do not use the latest, modern, and more complete nuclear reaction data and simulation tools. In fact nuclear data libraries, such as the Talys Evaluated Nuclear Data Libraries (TENDL), of which TENDL-2015 [5] is the most recent, are constantly changing, and so it is important that such scoping exercises can be easily and quickly reproducible – then they can be completed and compiled into a report shortly after a new library version release. Thus, significant effort has been expended in creating a largely automated computational platform, capable of performing the tens of thousands inventory simulations required, and collating them into a single report. Note that the conceptual designs of (DEMO) fusion reactors, particularly within the European research programme, are also evolving, and so the ability to repeat these material scoping studies quickly and automatically allows a database to be produced for the most recent engineering designs (although most design changes only impact significantly on deep – relative to the plasma – regions of the DEMO vessel, where changes in near-plasma regions can have an impact on the neutron fields in those deeper regions, and will have less effect on the database of results for plasma-exposed first wall conditions discussed in this paper).

This paper describes a comprehensive scoping study of the activation, transmutation and primary damage (PKA) characteristics of all naturally occurring elements from hydrogen to bismuth under typical irradiation conditions predicted for the plasma-exposed first wall (FW) of a DEMO power plant. Naturally-occurring U and Th actinides are not considered for the present databases because the additional processing needed to properly handle the fission yields is not currently included in the automated infrastructure. The required inventory simulations were performed with FISPACT-II [2,3] and TENDL-2015 [5], together with a modern nuclear decay data file, UKDD-12 (built from EAF-2007 decay data [6] with inclusion of some updates and an increased set of short-lived nuclides to cover the advancements in TENDL). These results are an update to the database already published in an openly available report [7], which was performed with the earlier TENDL-2014 [8] nuclear library and provides a global picture of the response of the elements, covering the majority of nuclear technological space, but focussing specifically on typical FW-DEMO conditions.

An important aspect to the scoping calculations is the ability to explore trends in particular nuclear observables, such as gas production rates, or shutdown activities. Thus, since it is not practical to present anything other than examples of the results presented

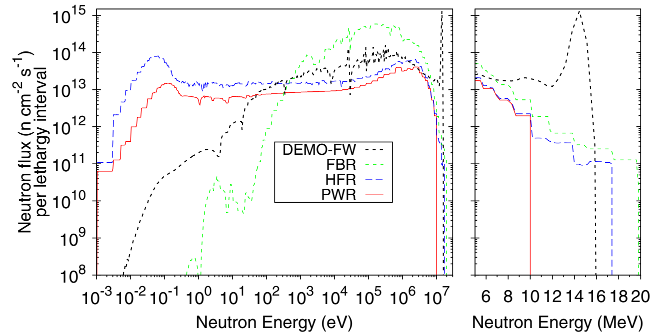

Fig. 1. The four neutron spectra used for the scoping calculations, where DEMO-FW is a typical first wall spectrum for a demonstration fusion power plant (total integrated flux of 5.9×10^{14} n cm^{-2} s^{-1}) [15,16]; FBR is the core assembly spectrum for the large-scale prototype fast breeder superphenix reactor that was located in the south of France (2.4×10^{15} n cm^{-2} s^{-1}); HFR is the spectrum for volume-averaged low-flux material test location of the high-flux reactor at Petten, Netherlands (5.3×10^{14} n cm^{-2} s^{-1}); and PWR is the fuel assembly-averaged spectrum for the type P4 pressurized-water reactor at the Paluel site in France (3.25×10^{14} n cm^{-2} s^{-1}). Left: the spectra on a logarithmic eV scale showing the full energy range. Right: a linear MeV scale, showing the high-energy parts of the spectra, in particular the fission tails.

in the report of the full database [7], here, instead, we focus on the comparison of certain DEMO-TENDL-2015 results for a nuclear-relevant subset of the elements. Furthermore we also compare the TENDL-2015 results with those calculated using other international, general-purpose nuclear cross section libraries: ENDF/BVII.1 [9], JEFF-3.2 [10], and JENDL-4.0 [11]. Additional databases [12–14] have also been produced for typical fission scenarios, and TENDL-2015 results from these are also discussed and compared against fusion equivalents.

2. Calculations and results per element

Fig. 1 shows the DEMO first wall (FW) neutron spectrum used for the main calculations in [7] with TENDL-2014 [8] and the updated ones with TENDL-2015 [5] in this paper, together with the three typical fission spectra used for the additional databases [12–14]. The DEMO model used to calculate this spectrum was produced in 2013 under the EFDA (now EUROFusion) European work programme on Power Plant Physics and Technology (3PT) [15,16]. The model has a simplified geometry with homogenised material mixtures and contains tritium-breeding modules based on a helium-cooled pebble-bed (HCPB) concept. It is part of a series of evolving DEMO concepts within the European design programme and the FW spectrum selected for the calculations is expected to represent the typical response for a material in a plasma-exposed region of a DEMO reactor. A new database has recently been produced with TENDL-2015 for a more recent European DEMO design, but the results presented in the associated report [17] are not significantly different from those presented here (and are not considered in the present work because they have not been repeated with the other nuclear libraries).

An automated script runs for each pure element, where the input composition is an element's naturally occurring isotopic composition (minor, but often unavoidable, impurity elements are not included), a set of irradiations with this DEMO spectrum (followed by cooling, as appropriate) using the FISPACT-II [2,3] inventory code, and produces the following outputs, which are fully described in [7]:

1. *Activation tables* – six tables, one for each of total (specific) activity (Bq kg^{-1}), decay heat (kW kg^{-1}), γ (contact) dose rate (Sv h^{-1}), inhalation and ingestion dose (Sv h^{-1}), and (IAEA)