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Mark R. Gilbert, M. Fleming, J.-Ch. Sublet



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Automated Inventory and Material Science Scoping Calculations under Fission and Fusion Conditions

Mark R. Gilbert, M. Fleming and J.-Ch. Sublet

United Kingdom Atomic Energy Authority, Culham Science Centre, Abingdon OX14 3DB, UK
mark.gilbert@ukaea.uk

Abstract - The FISPACT-II inventory simulation platform is a modern computational tool with advanced and unique capabilities. It is sufficiently flexible and efficient to make it an ideal basis around which to perform extensive simulation studies to scope a variety of responses of many materials (elements) to several different neutron irradiation scenarios. This paper briefly presents the typical outputs from these scoping studies, which have been used to compile a suite of nuclear physics materials handbooks, providing a useful and vital resource for material selection and design studies. Several different global responses are extracted from these reports, allowing for comparisons between materials and between different irradiation conditions. A new graphical output format has been developed for the FISPACT-II platform to display these “global summaries”; results for different elements are shown in a periodic table layout, allowing side-by-side comparisons. Several examples of such plots are presented and discussed.

I. INTRODUCTION

With the current maturity in nuclear inventory simulations it is also important to improve the way the results from the extensive output data sets are processed, analyzed and presented. In the past, only small amounts of data have been presented, usually for only one or two irradiation scenarios for a select few materials. Nowadays it is possible and routine to perform scoping calculations for many materials, for example the entire periodic table of elements, in multiple irradiation environments. The resulting data is vast and requires careful handling if the information is to be disseminated in an understandable and consistent manner. For this reason, the UKAEA, over a period of several years, has developed a suite of computational techniques that integrate with its own internationally recognised, modern inventory simulation platform FISPACT-II [1, 2]. These produce a variety of useful visual outputs to represent as much of the data as possible from single or multiple inventory simulations. This has culminated in the production of automatically-generated validation and verification reports [3, 4, 5] for the latest, modern nuclear data libraries TENDL-2015, ENDF/B-VII.1, JEFF-3.2 and JENDL-4.0u, as well as a new generation of extensive nuclear-physics materials handbooks [6, 7, 8, 9, 10, 11]. These handbooks, in particular, provide a huge wealth of information, scoping the radiological, transmutation (burn-up), and primary damage function responses for materials in typical fission reactor and predicted fusion environments. Furthermore the automated infrastructure, which efficiently creates and processes the tens of thousands of FISPACT-II & library inventory simulations required for the handbooks, can also be used to perform comparison studies by extracting the same response metric from the results of each material in a handbook and across multiple handbooks for nuclear library and/or environment. In this paper we briefly present the structure of the handbooks, before focussing on these comparisons for different response metrics.

II. CALCULATIONS AND PRESENTATION

For each handbook, an automated script runs, for each element or material, a sequence of simulated irradiations (followed by cooling as necessary) are performed for a set of incident neutron irradiation spectra (but focussing on one “main spectrum” for many outputs) using the FISPACT-II inventory code, and produces the outputs described below, which are fully described in, for example, [6]. Note that all results shown in the various example plots, and elsewhere in this paper, were

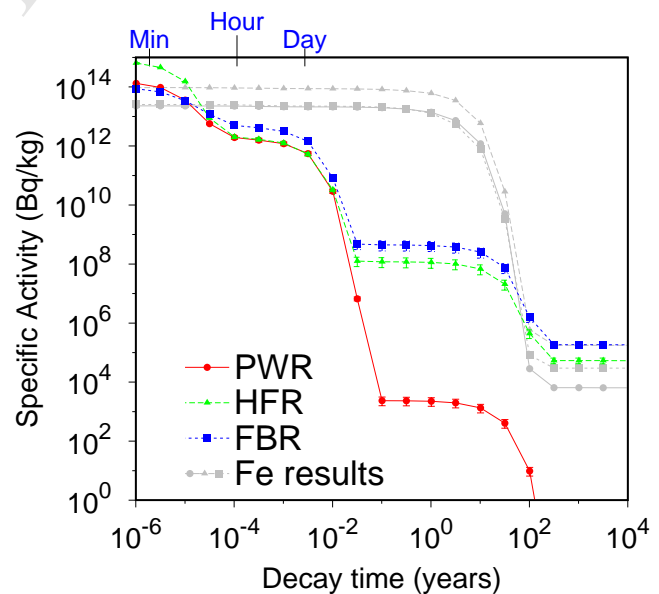


Fig. 1. Decay-cooling response of pure aluminium following 2 full-power year (fpy) irradiations under 3 typical fission scenarios: pressurized water-cooled reactor (PWR), the high-flux reactor (HFR) at Petten, and a fast-breeder reactor (FBR). The neutron flux spectra used are shown and described in more detail in Figure 3.

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