Inertial Fusion Reactor Physics: effect of Activation and Radiation Damage of Materials, and Tritium emissions

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1. Activation of Materials: Safety and Environmental Issues

The ACAB system [1] to compute the inventory evolution as well as a number of related inventory response functions useful for safety and waste management has been used by Lawrence Livermore National Laboratory (LLNL) for the activation calculation of the National Ignition Facility (NIF) design as well as for most of the activation calculations, S&E studies of the HYLIFE-II and Sombrero IFE power plants with a severe experimental testing at RTNS-II of University Berkeley. Pulsed activation regimes can be modelled (key in inertial confinement fusion devices test/experimental facilities and power plants), and uncertainties are computed on activation calculations due to cross section uncertainties. In establishing an updated methodology for IFE safety analysis, we have also introduced time heat transfer and thermal-hydraulics calculations to obtain better estimates of radionuclide release fractions. Off-site doses and health effects are dealt with by using MACSS2 and developing an appropriate methodology to generate dose conversion factor (DCF) for a number of significant radionuclides unable to be dealt with the current MACSS2 system. We performed LOCA and LOFA analyses for the HYLIFE-II design. It was demonstrated the inherent radiological safety of HYLIFE-II design relative to the use of Flibe. Assuming typical weather conditions, total off-site doses would result below the 10-mSv limit. The dominant dose comes from the tritium in HTO form. In the Sombrero design, a severe accident consisting of a total LOFA with simultaneous LOVA was analysed. Key safety issues are the tritium retention in the C/C composite, and the oxidation of graphite with air that should be prevented. The activation products from the Xe gas in the chamber are the most contributing source to the final dose leading to 47 mSv. We also analysed the radiological consequences and the chemical toxicity effects of accidental releases associated to the use of Hg, Pb, and

Be, as IFE materials under HYLIFE-II framework scenario. For those three materials, the chemical safety requirements dominate strongly over radiological considerations. Also, the role of clearance as waste management option for HYLIFE-II was explored. For the confinement building, which dominates the total volume of the waste stream, all the material could be released from regulatory control for unconditional re-use after about one year of cooling following plant-shutdown. Different applications in assessing the impact of cross section uncertainties are undertaken. In regards to NIF [2], we focused on the activated concrete-gunite outer shell of the reaction chamber. It is found that current cross sections allow a reasonably confidence in the results. Regarding IFE [3], it is proved the important effect of activation cross-section uncertainties on that the waste management assessment of different types of steels for the HYLIFE-II reactor. The necessary improvement of some W and Nb cross sections is justified. On the other hand, in regards to magnetic fusion energy (MFE) [4], we addressed the activation performance of the outboard first wall (FW) of a demonstration (DEMO) reactor. The critical cross sections to be improved are $(n,\gamma-m)$ for the isotopes 59 Co and 93 Nb in the keV energy range.

2. Radiation Damage of Fusion Materials

Ferritic-Martensitic Steels (including Oxide Dispersion Strength, ODS, technique), Composites based in SiC, and Vanadium alloys are materials presently under discussion as structural materials, together with C, Be, W, as first wall and some ceramics (silica, diamond, alumina) as optics and insulators. A systematic experimental program is pursued in different countries to assess their performance under the specific conditions they will be working on. It is very certain that a large and new irradiation facility is critically needed. International Fusion Materials Irradiation Facility (IFMIF) will cover such role. In the present time also Multiscale Modelling (MM) is getting a large role in obtaining predictive characteristic and defining the needed experiments. A common methodology work appears for fusion programs but also for nuclear fission (advanced Reactors/Generation IV and Accelerator Driven Systems for Transmutation) with coincidences in some of the materials. Key value has the validation of MM against specific experiments step by step at the microscopic and macroscopic levels and real understanding of damage processes, including effects of alloying and impurities elements. Microscopic parameters (using Molecular Dynamics, MD) which identify the effect of irradiation through new defects formation and diffusion, are being generated for some specific metallic materials (Fe, binary alloys FeCr, FeCu, V...) and their diffusion conducted by MonteCarlo [5]. Next step is being their interaction with dislocations (Dislocation Dynamics) and study of nucleation in the presence of He. That effect of He in FeCr alloys is certainly critical. We also derive macroscopic magnitudes using small-scale MM models in short simulation times by using MD defect-dislocation studies under stress [6]. We modelled pulse radiation damage, and we progress in the microscopic validation of Multiscale Modelling with experiments using pure and ultra-high pure Fe (effect of impurities) through a National Simulation-Experimental Program using ion irradiation [5]. Our work is also being concentrated in two IFE key materials (SiO₂/optics, SiC/low activation advance material). A MD tight binding scheme has been fully developed for β-SiC to understand the microscopic phenomena of the native defects and its diffusion at different temperatures. We reach an extraordinary good agreement among our calculated defects energetic and those results obtained using sophisticated and expensive method such as abinitio at 2000K [7]. MD is also being used to study the defects produced in fused silica by energetic atoms, neutron and gamma irradiation. We determine the structure factor, the bond angle distribution, co-ordination and ring statistics, and we conclude very good agreement with measurement of generation of fused silica glass [8]. Threshold displacement energies have been computed as a function of the direction of movement of PKA, and cascades of 5 keV are being actually extended to 10 keV. Two modelling-experimental programs have been started with CIEMAT for Silica analysis, to be extended to Alumina as first wall and ceramics insulators.

3. Tritium atmospheric diffusion and Environmental Pathways to human chain

A large and completely new work has been performed in the analysis of consequences of tritium release according with expected source emission from IFE Conceptual Reactors and others nuclear systems [9]. Key aspect here is to consider all chemical forms of tritium (HT and HTO) and their conversion to Organically Bound Tritium (OBT) with soil processes and consequences of re-emission to atmosphere. We report several important conclusions for the primary and, namely, secondary phases of tritium transport in the environment with final consideration of different time-dependent phases in dosimetry. Our new approach allows a more realistic simulation, and significant more restrictive limit in tritium handling as classically assumed in conceptual systems. This methodology has been successfully used in the work performed for establishing Vandellós site for ITER (EFDA Contract). The whole study of secondary phase drives to the conclusion that the behaviour of the tritium should be simulated using two well-differentiated studies: deterministic and probabilistic. Deterministic calculations are based on "a priori" fixed meteorological data, where the speed and directionality of the wind, class of atmospheric stability and rain intensity, as well as the boundary conditions to the atmospheric discharge (soil type, humidity of the air, temperature,

solar intensity) are given. The probabilistic study is based on measured real meteorological analysis every hour, and the probability that individuals can present dose for internal irradiation of the tritium is considered. Our conclusion is that these probabilistic studies provide the real dynamics of the processes, which are different from deterministic case. The effect of formation of OBT is concluded of key importance.

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