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The development of a fusion specific depletion interface code—FATI

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HIGHLIGHTS

- A new depletion code, FATI, has been developed for fusion applications.
- The code has been benchmarked against another well tested/benchmarked code, VESTA.
- The FATI code incorporates fusion specific features which are not present in current fission oriented depletion codes such as MONTEBURNS and VESTA.

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ABSTRACT

Knowledge of nuclide burn-up within lithium blankets has a crucial part to play in the safety, reliability and feasibility of a fusion reactor. A new depletion interface code is presented called FATI (Fusion Activation and Transport Interface) which interfaces MCNP with FISPACT. The intended primary application of FATI is the simulation of nuclide burn-up within fusion reactor blankets. This paper describes some of the functionality of FATI and presents a comparison of percentage variation of the nuclide atomic densities, for a simple spherical blanket model, calculated by FATI and VESTA. The inventories of the two depletion interface codes differ by less than 1% for lithium and lead isotopes, while H and He isotopes differ by larger amounts due to variations in the methods used to model gas production in FISPACT and the PHOENIX burn-up codes.

1. Introduction

The performance, economic viability and safety of a fusion energy device are reliant on the component design and material composition since neutron fluences in a fusion device will be very high. Material compositions will change during the reactor's lifetime due to induced activation and nuclear decay of isotopes that are present. The modelling of the material composition during and after the fusion energy power plant's operational lifetime is required for radiation damage assessment, radioactive waste disposal and reactor efficiency. One of the most important issues which needs to be addressed in order to ensure fusion energy becomes sustainable and economical is the capability for on-site breeding of tritium. Considering that a 1 GW fusion reactor would need a tritium refuelling rate of at least 184 g/day, there is no large natural source of tritium on earth and that the world's entire civil tritium inventory (~22 kg [1]) could not sustain a single fusion reactor operation for more than a few months operation. It is vitally important to produce enough tritium to sustain the reactor, however it is also important not to over-produce tritium due to economic and safety considerations.

Many tritium breeding concepts have been put forward to solve this issue, however the most promising solution is the concept of a tritium breeding blanket which surrounds the fusion reactor. In some concepts a lithium containing blanket of 40–60 cm depth is placed around the reactor which absorbs fusion neutrons and produces tritium primarily via the ^{6}Li(n,α)T and ^{7}Li$(n,\alpha n\prime)$T reactions. The rate of burn-up of lithium in any blanket concept needs to be modelled accurately in order to ensure the design is capable of constantly producing tritium at a rate which is greater than the rate of tritium usage plus tritium losses. The time-dependent generation of tritium can be addressed using neutronic simulations combined with control theory approaches. For instance, lithium ceramic breeders require helium purge gas to remove tritium from the blanket [2] and flowing liquid Li–Pb breeders require online purification [3].

The modelling of material composition and tritium breeding rates can be achieved with depletion analysis, which involves the modelling of neutrons throughout the reactor geometry, the nuclear reactions which they initiate and subsequent nuclear reactions. Several depletion codes were developed primarily for the

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fission industry and do not inherently possess all capabilities required to model some aspects of fusion systems adequately; notably the many additional energy threshold reactions which are possible in a fusion environment due to the high energy neutron source. Therefore the primary objective of writing a new depletion interface code, when other fully tested and comprehensive depletion codes already exist is to create a depletion code that is capable of modelling systems that are specific to fusion devices.

The time dependent behaviour of nuclear systems can be modelled with coupled Boltzmann transport [4] and Bateman equations [5]. Although the Boltzmann–Bateman system is closed and it describes a nuclear system well theoretically, it is not practical to solve this system in its current form. The cross-sections are energy dependent, as such they can be described in the multi-group format as several thousand cross-sections corresponding to a specified energy group structure. Recent burn-up studies [6,7] have shown that a minimum of 43,000 energy groups are required for fission burn-up studies and a minimum of 16,000 energy groups are required for fusion burn-up studies. At present, deterministically solving a Boltzmann–Bateman system with more than 16,000 energy groups is beyond the capabilities of most computer clusters and supercomputers. This is mainly due to limited RAM and a lack of codes that are capable of spatial and energy decomposition. For this reason, a hybrid stochastic–deterministic solver is preferable, where the transport is solved via Monte Carlo (MC) methods and the Bateman equations are solved deterministically. The stochastic (MC) method is less computationally demanding for complicated 3D geometries, such as fusion reactors, and allows the neutron spectra to be determined with an arbitrary number of bins. No complete hybrid stochastic–deterministic solver exists, however several depletion linker codes have been developed that link MC transport codes and Bateman solvers. The list of such codes include VESTA, MONTEBURNS [8], MOCUP [9], BGCORE [10]. A new depletion interface code is sought in order to meet the depletion requirement of fusion systems. Currently available depletion interface codes have a fission oriented modus operandi. Thus, these codes are over-specified in some areas, such as criticality calculation tools. They are also underspecified in some ways such as the inherent lack of ability to calculate tritium breeding ratios/inventories and lack of relevant cross-section data (proton, deuteron, triton, alpha activation). A new depletion interface code, FATI (Fusion Activation and Transport Interface), has been written in order to meet the requirements of fusion systems.

2. Depletion linker-code theory

Radiation transport codes and burn-up codes are important tools used for reactor analysis, however they are both to some extent limited. Burn-up codes such as FISPACT [11] and ORIGEN [12] are able to calculate nuclide inventories over time, but are point codes. On the other hand, Monte Carlo radiation transport codes have the ability to resolve reaction rates and neutron spectra spatially, but not temporally in terms of activation/burn-up. The primary function of a depletion linker-code is the calculation of nuclide inventories with time and space by combining the functionalities of burn-up and radiation transport codes. This is achieved by solving radiation transport and burn-up problems in a manner which is similar to solving coupled differential equations. Firstly, a radiation transport run is performed to calculate reaction rates and neutron fluxes within each component of the reactor. For each reactor component, a set of reaction rates and/or fluxes are passed to the burn-up code to advance the nuclide composition with time as a result of neutron irradiation. Following burn-up calculations for selected components in the reactor, the new nuclide compositions are then passed back to the radiation transport code and the cycle is repeated until a required period of time has elapsed. The coupling can be performed by utilising time-stepping routines with a specified order of accuracy, depending on the computational power and accuracy required. The simplest time-stepping routine for coupling the transport and burn-up equations is the forward Euler method:

$$\underline{\Phi}_c^n = \mathbf{M}(\underline{N}_c^n) \tag{1}$$

$$\underline{N}_c^{n+1} = \mathbf{B}(\underline{\Phi}_c^n, \underline{N}_c^n, \Delta t), \tag{2}$$

where the operator, **M**, is the Monte Carlo transport operator which for a specified nuclide set, $\underline{N}_c^j$, relating to cell, c, returns a set of reaction rates and/or neutron spectra, $\underline{\Phi}_c^j$. The operator, **B**, is the burn-up operator, which advances a given nuclide set, $\underline{N}_c^n$, forward in time by Δt.

This first-order method is acceptable provided the time-steps are small. However, second-order methods such as the mid-point method can be implemented in order to achieve a greater accuracy:

$$\underline{\Phi}_c^n = \mathbf{M}(\underline{N}_c^n) \tag{3}$$

$$\underline{N}_c^{[n+1]} = \mathbf{B}(\underline{\Phi}_c^n, \underline{N}_c^n, \Delta t) \tag{4}$$

$$\underline{\Phi}_c^{n+1} = \mathbf{M}(\underline{N}_c^{[n+1]}) \tag{5}$$

$$\underline{N}_c^{n+1} = \mathbf{B}\left(\frac{1}{2}(\underline{\Phi}_c^n + \underline{\Phi}_c^{n+1}), \underline{N}_c^n, \Delta t\right) \tag{6}$$

The first set of reaction rates, $\underline{\Phi}_c^n$, calculated by the mid-point rule will be underestimated while the second set, $\underline{\Phi}_c^{n+1}$, will be over estimated. Thus, the average of the two sets of reaction rates is considered to be a good approximation. An alternative to the averaging of reaction rates, is the predictor–corrector algorithm which calculates reaction rates half-way through the time-step and completes a burn-up step for a whole time-step based on the half-step reaction rate.

Third and fourth order methods can be implemented, however higher-order methods are not commonplace for two reasons. Firstly, the increased computational cost of completing more than two Monte-Carlo runs per time-step is not guaranteed to increase the accuracy of the solution. This is due to the limitation of the Monte-Carlo calculation which computes its solution with an order of accuracy of 1/2 [13]. The second, more problematic effect of higher-order methods is the increased computational cost of performing several Monte-Carlo runs per time-step. The Monte-Carlo simulations are often extremely computationally expensive and are typically accountable for greater than 95% of the computational power of the depletion analysis. Depletion analysis, based on second-order methods can take several days/weeks to run on modern computer clusters, hence a further increase in computational cost is, in most scenarios, often viewed as being prohibitively expensive.

An alternative approach to conventional time-stepping is the rate extrapolation technique (RET), which is implemented in FATI. The majority of the computational expense incurred by performing a burn-up calculation can be attributed to the MC radiation transport steps. The main task of each transport step is the direct/indirect calculation of reaction rates, $\overline{\sigma\phi(t)}$, in each cell via pointwise/multigroup methods. As these reaction rates are governed by burn-up the general form of each reaction rate solution will have an exponential form. Given that the burn-up, over the lifetime of the fusion reactor, is generally only 5–10% an approximation of the exponential form can be made in order to reduce the number of MC steps. Truncating the exponential Taylor series expansion to just first order results in the general form of the