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Development of time-dependent reaction rates to optimise predictor–corrector algorithm in ALEPH burn-up code

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ABSTRACT

Shells coupling Monte-Carlo transport and deterministic depletion codes are extensively used in the nuclear field to simulate material changes throughout irradiation. The dynamic behaviour of the phenomenon is described by the system of coupled ordinary differential equations, with generally a stiff matrix of coefficients that current codes keep constant in time along each burn-up interval. The matrix coefficients represent decay constants and microscopic reaction rates of the numerous nuclides involved in the calculations. For a typical burn-up problem, their determination consumes most of the required computational time while only a small fraction is spent by the depletion solver. Predictor–corrector methods have been implemented to guarantee more accurate results, but not much has been done to overcome the running time issue.

This work presents a unique and innovative feature of the ALEPH Monte-Carlo burn-up code which optimises the depletion algorithm by using time-dependent matrix coefficients. Linear polynomials interpolate the evolution of the matrix coefficients along a few consecutive time steps. Then, trend curves are constructed and used to extrapolate the effective reaction rates in the following intervals, thus reducing the total required computational time spent in the neutronic calculations. This technique has been implemented in the version 2 of the ALEPH Monte-Carlo burn-up code and validated against the REBUS experimental benchmark. The results revealed a considerable computational time saving without any drawbacks in the accuracy.

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1. Introduction

Calculating isotopic inventories has become of primary importance in all nuclear systems concerning safety-related aspects, operation and waste management purposes. In addressing this task, appropriate burn-up calculation codes (also known as depletion, or inventory codes) have been developed worldwide. The spread of coupled Monte-Carlo burn-up codes came along together with the growth of computing power that allowed a wide share and development in nuclear reactor applications and nuclear criticality research.

The Monte-Carlo burn-up code ALEPH is being developed at SCK•CEN since 2004 (Haeck and Verboomen, 2006). However, already 30 years ago stochastic transport codes have been coupled with material depletion solvers. Indeed, the Monte Carlo particle transport code MCNP (Booth et al., 2003) has been linked with the one-group depletion code ORIGEN (Croff, 1980) in automatic running programs such as MCODE (Xu et al., 2002), MONTEBURNS (Poston and Trellue, 1999) or MCOR (Tippayakul et al., 2006). Also the ALEPH code figures in the list, as it combines any version of MCNP (Briesmeister, 2000) or MCNPX (Pelowitz, 2008; Pelowitz, 2010) Monte-Carlo radiation transport codes with the ORIGEN-2.2 (Croff, 1980) depletion code, in its first release, and the RADAU5 module (Hairer and Wanner, 1996) in the newer version ALEPH2 (Stankovskiy and Van den Eynde, 2011).

Burn-up Monte-Carlo codes merge the potentials of a stochastic Monte-Carlo transport code and a deterministic solver. The Monte-Carlo tool solves the Boltzmann transport equation by stochastic Monte-Carlo method which owes the accuracy of its results to the amount of histories simulated to derive the statistical behaviour of the system. Stochastic codes return the most accurate, locally dependent, spectra and fluxes in realistic three-dimensional geometries.

Monte-Carlo codes reproduce the spectrum calculation even in complex full 3D geometries, but they show evident limits in applicability to follow the time-dependent behaviour of the neutronic parameters. Therefore, depletion solvers have been developed to simulate the dynamic evolution of the isotopic densities subject

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to irradiation. Amongst them, several tools can be mentioned like CINDER'90 (Wilson et al., 1997) and ORIGEN, or its updated version ORIGEN-S which is part of the SCALE code system (Gauld, 2009). However some codes use built-in burn-up depletion modules as MCB (Pusa and Leppänen, 2010) or the CRAM (Cetnar et al., 2006) algorithm of SERPENT (Leppänen, 2010).

Numerical methods are extensively used to perform these calculations, such as the matrix exponential technique by series expansion in ORIGEN-2.2, while the RADAU5 module, recently added to ALEPH2 to replace ORIGEN-2.2, utilises the implicit Runge–Kutta method RadauIIA (3 stages, accuracy order 5) (Xie, 2011). In fact, it has been known to have a high order of accuracy of the outcomes and excellent stability properties in solving stiff ordinary differential equations (Stankovskiy and Van den Eynde, 2012).

The dynamic evolution of the irradiated material is modelled by a system of ordinary differential equations (ODE's), where the governing parameters are all the reaction rates involved in the system, and are clustered in a square and sparse matrix of the coefficients. The irradiated nuclear fuel includes thousands of different nuclides with widely varying reaction rates, resulting in an extremely large and stiff matrix. Besides, the matrix coefficients are strongly dependent on isotopic compositions and vice versa as they affect each other leading to very complex combined problems.

In the previous statement, as well as in the following of this article, the "reaction rates" are considered as microscopic instead of macroscopic, therefore are measured in (s^{-1}) instead of the customary (atoms/s) unit.

Since burn-up calculations focus on long-term variations of the irradiated materials, the neutronic part and the depletion of material compositions are solved in sequence in order to decouple the problem. First the MCNP part calculates the particle flux in steady-state conditions as it adverts to the nuclide concentration at the beginning of the interval. Then, the numerical solver burns the materials keeping constant the matrix of the coefficients. This procedure is extensively used in most of the currently available burn-up codes, including ALEPH1 and ALEPH2. Although their large diffusion, such codes are considerably weak on the CPU time consumption point of view. In fact, the difference in running time between the two subdivisions is remarkable: for a typical burn-up computation the most of the time is spent to perform the neutronics, while only several percents of the total time are consumed to deplete the material.

The work described in this paper aims at overcoming the time consumption issues by modifying the nature of the solution procedure. Thus, the matrix coefficients are assumed linearly dependent on time throughout the whole burn-up interval as they might better reproduce the stiffness of the system.

The technique adopts polynomial functions to interpolate selected matrix coefficients along consecutive time intervals, with the retrieved curve extrapolating the reaction rate values in the following steps. The interpolating feature allows to skip some of the time-expensive Monte-Carlo transport calculations as the reaction rates are instead predicted by linear curves.

The foreseen results expect a comparable or even higher accuracy on the isotopic inventory at the end of calculations due to the improved reproduction of the matrix evolution in time. Moreover, since MCNP(X) calculations are severely reduced in number, the computational time is supposed to decrease.

2. Methodology

2.1. ALEPH working scheme

A typical ALEPH calculation starts with the processing of the input file—see Fig. 1. The ALEPH input file is generally straightforward and easily comprehensible as it wraps around the MCNP(X) input file and requires only some extra cards.

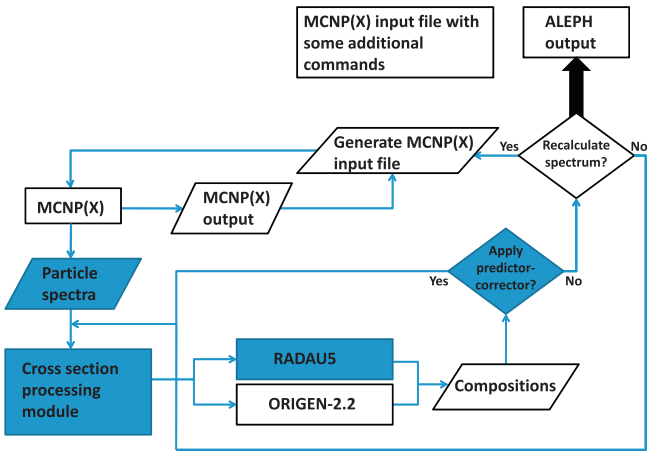

Fig. 1. Calculation flow inside ALEPH2.1 (Stankovskiy and Van den Eynde, 2011). Highlighted boxes were not present in the previous version ALEPH1.1.3.

As the computation begins, ALEPH builds a new MCNP(X) input file based upon the input options of the user and starts the MCNP(X) calculation. The MCNP(X) code determines the flux distribution in every burn-up zone at the beginning of the burn-up interval as it resorts to stochastic Monte-Carlo method. Afterwards, the ALEPH code uses the neutron spectra for the different irradiation zones to collapse, in combination with the evaluated nuclear data library, the total spectral-averaged single-group microscopic cross sections $[\bar{\sigma}]$ and the integrated flux $\bar{\varphi}$.

The determination of the reaction rates $[\bar{\sigma}]\bar{\varphi}$ comes from an optimal, highly accurate multi-group binning approach, while the one-group averaged flux $\bar{\varphi}$ is computed either normalising it to the power or normalising the source strength to the results of the selected tally requested in the MCNP(X) part of the input file (Stankovskiy and Van den Eynde, 2011). All the parameters are then gathered together with the decay constants $[\lambda]$ in the matrix of the reaction rates

$$[\boldsymbol{A}] = [\bar{\sigma}]\bar{\varphi} + [\lambda] \tag{1}$$

and then uploaded in the ODE's system

$$\frac{d\boldsymbol{N}(t)}{dt} = [\boldsymbol{A}]\boldsymbol{N}(t) \tag{2}$$

which models the dynamics of the isotopic inventory evolution throughout the time step. $\boldsymbol{N}$ turns out to be the M-vector of nuclide concentrations and $[\boldsymbol{A}]$ is the generally $M \times M$ stiff square matrix of the coefficients as M is the number of nuclides involved in the calculation. Alternatively, one can rewrite each equation in the extended form

$$\frac{dn_m(t)}{dt} = \sum_{n \neq m} a_{mn} n_n(t) - a_{mm} n_m(t) \tag{3}$$

where the matrix coefficients cluster all the neutronic contributions. Respectively, a_{mm} are the disappearance rates of nuclide m, which belong to the main diagonal of the matrix $[\boldsymbol{A}]$ and give no contribution to the coupling of the system, while the coefficients a_{mn} are the production rate of nuclide m from nuclide n and loosely couples the equations.

The current implementation of ALEPH calculates these reaction rates at the beginning of each time interval as they are assumed to be constant along the time step (see Fig. 2). However, the neutron flux spectrum and the cross sections present a dependence on the time, therefore the assumption of constant matrix coefficients is

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