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ACTYS-1-GO: A faster and accurate algorithm for multipoint nuclear activation calculations

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ABSTRACT

This article reports a relatively fast and accurate algorithm to solve large sized nuclear activation problems in one single run. The present algorithm reads material definition and neutron flux spectra generated by transport codes for complex geometries and then performs activation calculation based on the common parameters of the problem. The mathematical and computational details of simultaneous multipoint activation problem are presented along with the solution strategies. The present algorithm speeds up such calculations by generating a common coefficient matrix for a compact subset of the problem, depending upon one or more radiological results expected from the analysis and then removing the sparsity of the cross-section matrix. The algorithm is implemented in a computer code named 'ACTYS-1-GO'. All the above steps and the implementation details are summarized in this article. A detailed validation of the code is also presented. Computational performance comparison for fusion-relevant problems has been carried out with the sequential use of activation code FISPACT and 'Fornax' module of Attila computer code.

1. Introduction

Nuclear activation study of structural material in fission or fusion device is very crucial from an operation, maintenance and safety point of view [1,2]. Materials installed in these devices face stringent regulations to minimize the damaging effects of neutron irradiation [3,4]. The structural materials should be able to withstand the neutron flux and fluence emitted from the core of the device. Also from a safety point of view, these materials should be able to tolerate accidental leakage of radiation as well [5,6]. This kind of rigorous nuclear activation analysis can only be achieved by the use of efficient activation codes [7,8]. These codes simulate neutron induced reaction and radioactive decay occurring in the materials, placed in a neutron environment. A number of radiological parameters including ShutDown gamma Dose Rate (SDDR) and radwaste classification are obtained through such analysis [9,10]. SDDR is the gamma dose rate emitted from the radioactive materials after the shutdown of the reactor/nuclear device. One of the major concerns of any nuclear device is the classification and disposal of radioactive waste produced in the device. An accurate estimation of radioactive wastes (radwaste) expected and its classification is required during the design of nuclear machines. This will help to achieve a better design based on various activation calculations and through a number of optimization procedures. Various classification strategies are used to segregate harmful radioactive waste from less harmful ones and then properly dispose of the waste [11,12]. Radiological quantities like SDDR, are used to calculate the lifetime of various components of the device for making the maintenance and dismantlement strategies. Thus commissioning of any nuclear device relies on an intricate nuclear activation calculation and analysis of the entire device and its components [13,9].

Neutrons produced within the plasma travel throughout the device. These neutrons may be absorbed or scattered on the way, changing the flux. Since the flux is not constant throughout the device, the resulting activation will also be different. So in order to calculate radiological responses, the device or the reactor is divided into smaller sections, meshes, depending upon the gradient in neutron flux. A trivial way to perform activation calculation and gamma source generation for many large devices is to call an activation code sequentially for each mesh or to perform calculations for many meshes in few steps using a dedicated algorithm [14,15]. In a multipoint calculation, the activation code considers the entire device as one single system and optimizes the activation calculation at each mesh by making use of common parameters for the material. Whereas a sequential code simply runs at each mesh irrespective of the problem at hand. Activation of a mixture of SS and

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H_2O for an irradiation period of 3 years with flux 1.3E11 $cm^{-2}\,s^{-1}$ takes ~2 s for FISPACT. Therefore for 1 million mesh, it is expected to take ~23 days. This kind of sequential run is computationally very expensive. Hence coarse meshing is done to save time and effort [16]. This, however, may not yield desirable results for radiological quantities in a device with large gradients of flux. Also, such calculations may lead to overestimation or underestimation of some important radiological parameters. This can cause problems in selection of shielding material and other preventive measures.

Specifically, a complete activation calculation is usually more laborious in the case of fusion devices [17,18]. Because of the huge volume of fusion device and large variation in the composition of structural materials, there is a high spatial variation of radiological quantities. For example, ITER is a 23,000 tonnes experimental fusion device constituting of more than 100 different materials [19,20]. Plasma diagnostics and other major components are intricately placed inside the tokamak [13]. This requires a detailed and highly spatially resolved activation calculation. Thus for a complete and accurate activation analysis, a methodical way of multipoint calculation is required.

At ITER-India (Indian domestic agency of ITER) a project is being carried out to develop suitable code suites for nuclear activation calculations, radiation waste classifications and material (for nuclear devices) optimization based on various radiological responses of the materials. As a first step, a single-point (for one flux) nuclear activation code called 'ACTYS' is developed, validated and used for few ITER calculations. The mathematical as well as numerical solution strategies along with detailed validations are summarized in [21]. Some of the results including rad-waste calculations using ACTYS and a comparison with FISPACT is reported in [13]. In the second step, a fast, accurate algorithm for simultaneous activation calculations at all meshes within the geometry is developed. The algorithm is implemented into a computer code called ACTYS-1-GO (ACTivation AnalYsiS in 1 Go).

This paper reports the mathematical details, solution strategies, computational performance and various validations of ACTYS-1-GO.

2. Mathematical model and computation details

2.1. General description

The nuclear activation problem is governed by first order linear differential equation, known as Bateman equation [22]. In a homogeneous, infinite and infinitely dilute material, the time evolution rate of nuclides can be written as [23]:

$$\frac{dN_i}{dt} = -(\lambda_{ii} + \overline{\sigma}_{ii}\Phi)N_i + \sum_{j\neq i}(\lambda_{ij} + \overline{\sigma}_{ij}\Phi)N_j \tag{1}$$

The first term on the R.H.S is the loss term for nuclide N_i. λ_{ii} is the total decay coefficient and $\overline{\sigma}_{ii}$ is the total average loss due to transmutation. Second term on the R.H.S is the gain term, the production of nuclide N_i from various other nuclides N_j. λ_{ij} is the decay of isotope N_j to isotope N_i and $\overline{\sigma}_{ij}$ is the average transmutation probability of isotope N_j to isotope N_i. The time evolution rate for all the isotopes in the material is a set of coupled first-order linear differential equations. Since λ_{ij} and $\overline{\sigma}_{ij}$ are independent of N_j, these can be written in a matrix form [24]:

$$\frac{d\mathbf{N}}{dt} = -\Lambda\mathbf{N(t)} \tag{2}$$

where $\mathbf{N}$ is the vector containing concentration of all isotopes at time t and Λ is matrix of coefficients given as $\Lambda_{ij} = \lambda_{ij} + \overline{\sigma}_{ij}\Phi$. The solution of above equation is:

$$\mathbf{N}(t) = e^{-\Lambda t}\mathbf{N}_0 \tag{3}$$

For all practical/calculation purposes, reaction cross section data is condensed into groups using the formula:

$$\overline{\sigma}_g = \frac{\int_{E_{gi}}^{E_{gf}}\sigma(E)\Phi(E)dE}{\int_{E_{gi}}^{E_{gf}}\Phi(E)dE} \tag{4}$$

where $\overline{\sigma}_g$ is the average condensed cross section for group g, $\sigma(E)$ is the reaction cross section at energy E, $\Phi(E)$ is value of fusion spectrum at energy E, E_{gf} is the upper bound of group stricture and E_{gi} is the lower bound for the group g. Further details of condensation and reaction cross section can be obtained from [21]. Like nuclear reaction cross section, neutron flux is also segregated into groups considering the neutron emission spectra from the source. Most common group structure for fusion device is 175 Vitamin-J group [25]. The multigroup cross-section and neutron flux is then used to construct coefficient matrix using the formula:

$$\Lambda_{ij} = \lambda_{ij} + \sum_g(\overline{\sigma}_{ij}^g * \Phi^g) \tag{5}$$

where λ_{ij} is the radioactive decay constant of the isotope j to i, $\overline{\sigma}_{ij}^g$ is the groupwise reaction cross section of the isotope j to i and Φ^g is the groupwise flux.

The typical coefficient matrix generated using Eq. (5) is usually very stiff and sparse [26]. The stiffness of the matrix is because of the large variation in decay constants of the radioactive isotopes. For single target nuclide with one step nuclear interaction, kinematically possible reaction can produce nuclides with atomic numbers $\leq Z$ of the target, while sequential reaction like (p, n), (d, n) and (α, n) produce additional nuclides with higher Z value [27]. As each isotope can produce only a handful of different isotopes, the resultant coefficient matrix has huge sparsity. For example, a matrix created for a mixture of stainless steel and water irradiated for 3 years with the flux of 1.30E+11 $cm^{-2}\,s^{-1}$, has a sparsity of 99.99%, as shown in Fig. 1. Fig. 1 represents a coefficient matrix Eq. (5) of size 2043 × 2043, where 2043 is the number of isotopes considered for the activation calculation in the code. Dark region corresponds to the non-zero value of transmutation probability $\sum_g(\overline{\sigma}_{ij}^g * \Phi^g)$ in the matrix. This sparsity makes it difficult to use conventional methods to calculate exponential of the matrix given by Eq. (3) [28].

Most commonly 3 main mathematical methods are used by the activation codes to model such a complicated physical system, they are time step based ODE solver, matrix exponential methods and linear chain method [23,29,15,21]. Details of these methods are given in [21] and is omitted here for the sake of brevity.

2.2. Multipoint calculation and solution strategy of ACTYS-1-GO

ACTYS-1-GO uses the same technique of ACTYS to solve a linear chain for a given flux but uses a robust algorithm to make it suitable for simultaneous multiple point calculations. The various techniques for single point activation solver are detailed in [21], some of the points required for this paper is summarized below.

In ACTYS-1-Go, to calculate the inventory of isotopes produced in a material at time t for any incoming flux Φ^g, first the coefficient matrix $(\lambda_{ij} + \sum_g(\overline{\sigma}_{ij}^g * \Phi^g))$ is generated. Then using the initial material composition and their transmutation and decay probabilities into other isotopes, concentrations of isotopes are calculated via chain method.

During the activation process, isotopes present in the material are converted into other isotopes via nuclear reaction. These second generation isotopes can further be converted into different isotopes via transmutation or radioactive decay (Fig. 2). Each branch signifies a radioactive decay or transmutation of parent isotope into daughter isotope. Isotope 'A' is the initial parent present in the material. It can decay or transmute into two daughter 'B' and 'C' forming branches. Isotope 'D' and 'F' can decay or transmute to same isotope 'E', such a process is called as cross linking. Isotopes 'G' and 'H' have finite probability of transmuting into one another forming a loop. This forms a complex activation tree with same isotopes created at different