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# ALARA: THE NEXT LINK IN A CHAIN OF ACTIVATION CODES

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## ABSTRACT

The Adaptive Laplace and Analytic Radioactivity Analysis [ALARA] code has been developed as the next link in the chain[b] of DKR[1-3] radioactivity codes. Its methods address the criticisms of DKR while retaining its best features. While DKR ignored loops in the transmutation/decay scheme to preserve the exactness of the mathematical solution, ALARA incorporates new computational approaches without jeopardizing the most important features of DKR's physical modelling and mathematical methods.[4] The physical model uses "straightened-loop, linear chains" to achieve the same accuracy in the loop solutions as is demanded in the rest of the scheme.[5] In cases where a chain has no loops, the exact DKR solution is used. Otherwise, ALARA adaptively chooses between a direct Laplace inversion technique and a Laplace expansion inversion technique to optimize the accuracy and speed of the solution. All of these methods result in matrix solutions which allow the fastest and most accurate solution of exact pulsing histories. Since the entire history is solved for each chain as it is created, ALARA achieves the optimum combination of high accuracy, high speed and low memory usage.

## I. INTRODUCTION

When designing any system with a large neutron flux, an important characteristic is the amount of induced activation expected in the system's components during operation, at the end of life and at various times after the shutdown of the system. Many codes have been written to perform such calculations for a variety of systems, from accelerators to fission and fusion reactors. The special conditions of fusion reactors, such as high neutron flux/fluence and pulsed operation, have led to several variations of these codes.

The calculation of induced radioactivity in the first wall, blanket and shield materials is an important task for the design and safety of fusion reactors. The neutron products of the D-T reaction induce radioactivity by interacting with and transporting through these materials with much higher initial energies and populations than those of fission reactors of similar power. The results of these radioactivity calculations are used extensively in safety and design analyses to determine such parameters as the nature of the radioactive waste, the amount of shielding required for radiologically sensitive components, and the decay heating after shutdown. Like other engineering calculations, the accuracy of the results is important; overly conservative approximations result in costly and complicated designs while liberal approximations result in safety and technical hazards to the operators, scientists, public and equipment.

To solve this problem a code must perform two steps. First it must model the physical system in time, space and isotopic composition, creating a system of linear first order ordinary differential equations [ODE's]. Second, the solution to this system of ODE's must be found using a computational technique. Both steps are non-trivial since the physical problem, while finite in time and space, is theoretically infinite in isotopic composition, and the resulting ODE's have characteristics which can make their efficient and accurate solution difficult. Other codes exist to solve this problem,[6,7] each combining different physical modelling philosophies with different mathematical methods, but unfortunately, none uses an optimum calculation for speed and accuracy.

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[b] DKR will be used to refer to the most recent version (Ref. 3) of the family of codes originating with Ref. 1.

ALARA is a computational tool for performing such calculations. Given a groupwise neutron flux, ALARA uses data from a variety of libraries to determine the altered composition of materials. From this altered composition, the activity, $\beta$-, $\gamma$-, and $\alpha$-heating are determined. In addition, a groupwise $\gamma$-ray source can be computed by ALARA to be used for the calculation of biological doses. Finally, if provided with an adjoint importance field based on flux-to-dose conversion factors and the gamma source distributions, ALARA can directly calculate the biological dose.

## II. DESIGN PHILOSOPHY

ALARA has been designed with three basic principles in mind: accuracy, speed, and simplicity. These three qualities have been maximized in ALARA after extensive research of the models involved in such calculations.[4,5] The methods used to model the physical system and to perform the mathematical solution are carefully combined to preserve or enhance the accuracy while accelerating the speed of solution.

The accuracy (and precision) of the final solution is affected both by how realistically the physical system is modelled and by which mathematical methods are employed for the final solution. When modelling the physical problem, two of the most important issues are how to deal with loops in the decay/transmutation scheme and how to truncate the infinite isotopic composition to a finite problem, the former having a significant impact on the mathematical method. By finding a physical approximation to the loops which retains problem accuracy and allows for quite simple and efficient mathematical methods, ALARA has broken the unwritten rule that realistic treatment of loops requires complicated/inefficient mathematical methods. The keys to ALARA's mathematical accuracy are the ability to adaptively choose the mathematical technique combined with the accuracy of those techniques. Two of the three mathematical techniques which ALARA employs are mathematically exact!

The speed of problem solution is greatly affected by which class of mathematical method is used. In particular, unless a matrix method is used to model a pulsed history, the time of execution will be greatly increased. ALARA uses such matrix methods, using techniques to solve the linear transformation of the initial isotopic composition to the final composition for each pulse and inter-pulse dwell period, and then multiplying these matrices to get a complete linear transformation for the entire history. The general philosophy was also designed, throughout, with speed in mind, resulting in decisions which have beneficial impacts on the execution time.

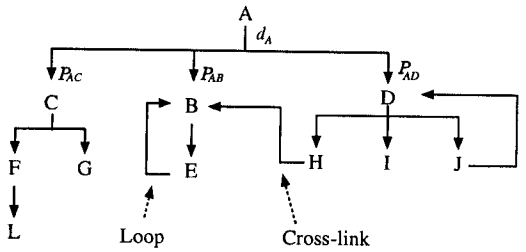


Figure 1: Basic Decay/Transmutation Scheme

While accuracy and speed have long been issues in the creation of engineering codes, it is becoming increasingly important that they are both easy to learn and simply maintained and adapted to new requirements. The code itself is designed to be more readable to future programmers and facilitate enhanced modularity. ALARA allows the user to find the solution to an activation problem in a variety of different multi-dimensional geometries, using a flexible system to define the material properties and allowing a complicated pulsed/intermittent irradiation history and a variety of after-shutdown solution times. Finally, through the use of a companion code, ALARA Data Conversion (ALARA_DC), ALARA is able to interface easily with neutron transport codes and use a variety of different data libraries (USACT93, EAF, etc.).

## III. PHYSICAL MODEL

As neutrons interact with the initial (usually stable) isotopes of a system, different isotopes are produced which, in turn, can decay or further interact with the neutrons, producing further isotopes, and so on, shown graphically in Figure 1. While this can be represented mathematically by a simple system of linear first-order ordinary differential equations, when loops exist in this decay scheme, the solution of this system is complicated. It is possible, however, to remove much of this complication by straightening the loops. That is, the loop is considered as an infinite number of subtrees, each containing the same isotopes as the loop (see Figure 2). When the mathematical system is viewed in a matrix representation, this process has the effect of converting a full matrix to a triangular matrix with repeated eigenvalues.

It is important to note that the subtrees resulting from such a loop, although described above as infinite, do not make the problem any larger. Modern data libraries are quite extensive which means that any problem, with or without loops, is effectively infinite in size and must be truncated based on some criteria. Choosing such criteria is not trivial since truncation results

in an approximation discrepancy which can best be described as "isotope loss". In the real system all isotopes have a finite probability of transmuting/decaying. When an isotope at the bottom of the model undergoes such a reaction, its product is lost from the system. The fraction of the initial isotope that passes through the branch leading to a particular isotope in question can be compared to a user defined tolerance. If this relative production at shutdown is greater than the tolerance, the branch will be continued; otherwise, it will be truncated. The only provision to this rule is when the relative production increases after shutdown, in which case all subsequent transmutation branches are truncated, but decay branches are followed until the full criteria are met. Such a truncation strategy will minimize the effect of this "isotope loss" caused by modelling errors.

Furthermore, since the straightened loops are truncated with the same rules as the rest of the tree, the error caused by loop straightening is bounded by the error from chain truncation. In particular, the truncation rules define the precision, or resolution, of the result while the truncation of loops affects the accuracy, or relative error, in the result. In all cases, the loop error will be less than the user-defined resolution of the result, and thus must be deemed insignificant. Analyses have shown that the inclusion of one or two iterations of a straightened loop leads to accuracies of less than $1 \times 10^{-6}$.[5]

## IV. MATHEMATICAL MODEL

Because loops have been straightened, the system of equations which represents the transmutation/decay scheme can be separated into individual chains to solve many small problems rather than a single large problem. Each of these problems is represented by a very simple system of first order ODE's which can be represented in matrix notation as

$$\dot{\vec{N}}(t) = \boldsymbol{C}\vec{N}(t) \tag{1}$$

where $\vec{N}(t)$ is the number density vector and $\boldsymbol{C}$ is a bidiagonal matrix,

$$\begin{bmatrix} -d_1 & 0 & 0 & \cdots & \cdots & 0 \\ P_1 & -d_2 & 0 & \cdots & \cdots & 0 \\ 0 & P_2 & -d_3 & \cdots & \cdots & 0 \\ 0 & 0 & P_3 & -d_4 & & \vdots \\ \vdots & \vdots & \vdots & & \ddots & 0 \\ 0 & 0 & 0 & \cdots & P_{k-1} & -d_k \end{bmatrix},$$

where $d_i$ is the destruction rate of the $i^{th}$ isotope and $P_i$ is the production rate of the $(i+1)^{th}$ isotope from the $i^{th}$. The general solution for this system is of the well known form

$$\vec{N}(t) = e^{\boldsymbol{C}t}\vec{N}_o(t).$$

In the trivial case where there are no loops, this system is solved analytically by the Bateman Equations, as is done in DKR. When loops do exist, however, there are repeated eigenvalues and other methods must be used. By transfering to the Laplace domain with parameter $s$, Equation 1 can be written as

$$\tilde{N}_i = \sum_{j=0}^{i} N_{j_o} \prod_{k=j}^{i-1} P_k \prod_{l=j}^{i} \frac{1}{s+d_l}, \tag{2}$$

which requires the inversion of the Laplace space function

$$\tilde{F}_{i,j}(s) = \prod_{l=j}^{i} \frac{1}{s+d_l}. \tag{3}$$

ALARA is then able to perform simple analysis of the chain which this matrix represents to adaptively determine which mathematical method is best suited to solve this problem quickly and accurately. If no loops exist, the standard Bateman Equations can be used. When loops do exist, the product of the matrix radius and the time can be used to choose between two Laplace space methods: $1/s$ expansion or direct inversion.

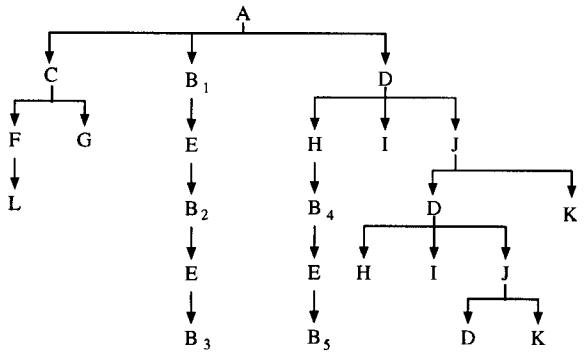


Figure 2: Straightened Decay/Transmutation Scheme

A. Laplace Expansion Method

For small radius-time products, $\tilde{F}_{i,j}(s)$ can be expanded as a series of $1/s$,

$$\tilde{F}_{i,j}(s) = \frac{1}{s^{i-j+1}} \left[ 1 - \frac{\sum_{l=j}^{i} d_l}{s} + \frac{\sum_{l=j}^{i} d_l \sum_{k=l}^{i} d_k}{s^2} - \frac{\sum_{l=j}^{i} d_l \sum_{k=l}^{i} d_k \sum_{m=k}^{i} d_m}{s^3} + \cdots \right]. \quad (4)$$

If $n = i - j + 1$, in the time domain, this becomes:

$$f_{ij}(t) = t^{n-1} \left[ 1 - \frac{t}{n!} \sum_{l=j}^{i} d_l + \frac{t^2}{(n+1)!} \sum_{l=j}^{i} d_l \sum_{k=l}^{i} d_k - \frac{t^3}{(n+2)!} \sum_{l=j}^{i} d_l \sum_{k=l}^{i} d_k \sum_{m=k}^{i} d_m + \cdots \right]. \quad (5)$$

B. Direct Inversion Method

On the other hand, for a small system, this problem might be solved exactly by hand by performing a Laplace inversion involving the Residue Theorem. For an arbitrary system, the necessity to find an arbitrary derivative, $\left[\tilde{G}^k_{i,j}(s)\right]^{(n)}$, of an arbitrary function, $\tilde{G}^k_{i,j}(s) = (s + d_k)^m \tilde{F}_{i,j}(s)$, could make the computational implementation of this Residue Theorem difficult. Due to the nature of this matrix, however, this differentiation can be implemented as a simple recursive function:

$$\left[\tilde{G}^k_{i,j}(s)\right]^{(n)} = \sum_{j=1}^{n} (-1)^j \left\{ \frac{(n-1)!}{(n-j)!} \left[\tilde{G}^k_{i,j}(s)\right]^{(n-j)} \sum_{l=1}^{i} \frac{1}{(s+d_l)^j} \right\}. \quad (6)$$

When this is used to invert $\tilde{F}_{i,j}(s)$ to the time domain, the solution can be found with mathematical exactness. (More complete derivations and analyses of the mathematics can be found in Reference 5.)

Using these methods, a matrix solution is found for a single irradiation pulse of the system. This is then multiplied by a matrix solution for a single interpulse dwell period and raised to a power to represent all the pulses.

## V. FUTURE ENHANCEMENTS

Many forms of enhancements are planned for ALARA in the future, most of which will result in greater versatility, user-friendliness and data handling capabilities.

- So that ALARA is easier to use in conjunction with other related codes, such as transport codes, a complete set of modules is being written to convert the data from those codes into the required format for use by ALARA.
- As new data become available, modifications can be made to account for the activation caused by sequential charged particle reactions in the materials.
- Much of the data already generated and used by ALARA can be used to provide enhanced pathway analysis, allowing a user to find the source of trace isotopes and radiation sources.
- As an even more sensitive method of determining initial sources of radioactive isotopes and trace elements, a "backwards" or "adjoint" activation calculation module will be developed. This will allow users to input particular isotopes of interest and have the code determine which initial isotopes will generate them and in what proportions. With this information, a user can quickly examine the sensitivity of the induced concentrations/activities to variations in the initial composition.
- Due to the nature of the problem solved by ALARA, it is a great candidate for parallelization. Efforts will be made to take advantage of this by creating versions which will operate under popular parallel computational environments.
- Finally, since the results are stored internally in their entirety, a post-processor will be attached to allow the user to view the results in a variety of formats and resolutions. Eventually, this will include functionality to display and print information such as production pathways, entire trees and numerical results in a graphical format.

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