Annals of Nuclear Energy 103 (2017) 163–172

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Development of an Application Programming Interface for Depletion Analysis (APIDA)

Daniel Lago, Farzad Rahnema *

Nuclear & Radiological Engineering and Medical Physics Programs, Georgia Institute of Technology, 770 State Street NW, Atlanta, GA 30332-745, USA

ARTICLE INFO

Article history:
Received 21 November 2016
Accepted 9 January 2017

Keywords:
Burnup
Benchmark
Bateman equations

ABSTRACT

A new utility has been developed with extensive capabilities in identifying nuclide decay and transmutation characteristics, allowing for accurate and efficient tracking of the change in isotopic concentrations in nuclear reactor fuel over time when coupled with a transport solution method. This tool, named the Application Programming Interface for Depletion Analysis (APIDA), employs both a matrix exponential method and a linear chain method to solve for the end-of-time-step nuclide concentrations for all isotopes relevant to nuclear reactors. The Chebyshev Rational Approximation Method (CRAM) was utilized to deal with the ill-conditioned matrices generated during lattice depletion calculations, and a complex linear chain solver was developed to handle isotopes reduced from the burnup matrix due to either radioactive stability or a sufficiently low neutron-induced reaction cross section. The entire tool is housed in a robust but simple application programming interface (API). The development of this API allows other codes, particularly numerical neutron transport solvers, to incorporate APIDA as the burnup solver in a lattice depletion code or reactor core analysis code in memory, without the need to write or read from the hard disk. The APIDA code was benchmarked using several decay and transmutation chains. Burnup solutions produced by APIDA were shown to provide material concentrations comparable to the analytically solved Bateman equations – well below 0.01% relative error for even the most extreme cases using isotopes with vastly different decay constants. As a first order demonstration of the API, APIDA was coupled with the transport solver in the SERPENT code for a fuel pin cell depletion problem. Results show APIDA to be effective and efficient in solving lattice depletion problems, in addition to being successful in terms of portability for users to implement via the API.

1. Introduction

The world's energy demands are at historic levels and the need for clean, sustainable, and dependable power is unquestionably at the forefront of modern society. Nuclear power is increasingly becoming the most powerful tool to combat the impending energy crisis, subsequently making adequate tools to safely operate nuclear reactors and accurately track the changes in fuel over the core lifetime vital to ensuring the advent of a new fleet of nuclear power plants.

The current push in nuclear reactor physics research is to create all-encompassing codes capable of capturing all the multiphysics present in the complicated core of a nuclear reactor – thermal hydraulics, material performance, radiation shielding, and kinetics being the most relevant. This study focused on the creation of a novel burnup module with sufficient modernization to couple with current and future neutron transport solution methods.

The utility developed in this study, the Application Programming Interface for Depletion Analysis (APIDA), is a standalone burnup solver with an interface accessible enough to be coupled with potentially any transport solver to form a lattice depletion tool or reactor core analysis code. The proceeding sections discuss the methods used to solve the burnup equations, the verification of the solver, the construction of an application programming interface, and the initial coupling with a transport solver to produce preliminary results.

2. Development of a burnup solver

Development of the burnup solver in the APIDA code involved studies into multiple linear chain methods and matrix exponential methods. Literature review and implementation of proof-of-concept algorithms led to the conclusion that the Chebyshev

* Corresponding author.
E-mail addresses: dlago3@gatech.edu (D. Lago), farzad@gatech.edu (F. Rahnema).

http://dx.doi.org/10.1016/j.anucene.2017.01.010
0306-4549/

Rational Approximation Method (CRAM) was the most effective and flexible method for solving burnup equations.

While CRAM, and inherently any numerical matrix solver, handles the requisite transition matrices in burnup problems well, it cannot be applied to nuclides that introduce zeros into the diagonals of said matrices. Consequently, a linear decay chain solver needs to be applied to solve for the time rate of change of nuclide concentration for those isotopes.

The APIDA tool is the result of combining the two preceding methods – a hybrid matrix exponentiation and linear chain solver for burnup problems. The following section briefly outlines the theory and foundation of CRAM. For a more complete analysis, the reader is encouraged to refer to the work done by Pusa and Leppanen (2010) and Pusa (2011).

2.1. Matrix exponential solver – CRAM

The phenomena governing the time rate of change of nuclide concentration can be formalized by the following general equation.

$$\frac{dN_i}{dt} = \underbrace{\sum_{j=1}^{m} b_{ij}\lambda_j N_j + \sum_{k=1}^{m} y_{ik} RR_k N_k}_{\text{Production}} \underbrace{-(\lambda_i + RR_i)N_i}_{\text{Destruction}} \qquad (1)$$

$$RR_i = \int dX \phi(X)\sigma_i(X)$$

N_i = atom density of nuclide i
λ_i = radioactive decay constant of nuclide i
$\sigma_i(X)$ = neutron absorption cross-section for nuclide i over phase-space X
$\phi\ (X)$ = neutron angular flux over phase-space X
b_{ij} = branching ratio of all other nuclides to nuclide i
y_{ik} = branching ratio for neutron absorption by other nuclides that lead to nuclide i

Eq. (1) shows the time rate of change of the concentration of nuclide N_i as a balance equation with the net result being the sum of the destruction and production of the nuclide of interest. The necessary assumptions in forming Eq. (1) are as follows: a homogenous medium; space-averaged and energy-integrated reaction rate over one energy group; sufficiently small time step to assume a constant flux. In most lattice depletion applications, these assumptions are acceptable and provide accurate solutions if utilized appropriately.

Production of N_i can result from the decay of another nuclide N_j into N_i with the probability of said reaction expressed by its associated branching ratio b_{ij}, or production can come from nuclide N_k participating in a reaction under the influence of a flux resulting in the production of nuclide N_i. Destruction of N_i is determined by two factors, both of which are dependent on the type of problem and isotope. If the nuclide is unstable, its decay probability (λ) determines the removal rate. If there is irradiation, implying a flux (ϕ), then the nuclide's reaction rate determines the removal rate. If both principles are appropriate, then the decay probability and reaction rate are summed to constitute the removal coefficient for the nuclide N_i.

In regards to the reaction types represented by the branching ratios in Eq. (1), the initial implementation of APIDA considered the reactions shown in Table 1. While not all encompassing, these equations constitute most of the neutron-induced reactions occurring in a nuclear reactor. Future work for APIDA will address implementation of all neutron-induced reactions.

Historically, matrix exponential methods have been applied with varied success in multiple fuel decay and transmutation codes.

For a chosen set of isotopes, Eq. (1) can be set up in matrix notation as follows,

Table 1
Decay modes and their associated reactions.

Decay Mode	Reaction
$(n,2n)$	${}^{A}_{Z}X + n \rightarrow {}^{A-1}_{Z}X + 2n$
$(n,3n)$	${}^{A}_{Z}X + n \rightarrow {}^{A-2}_{Z}X + 3n$
$(n,4n)$	${}^{A}_{Z}X + n \rightarrow {}^{A-3}_{Z}X + 4n$
(n,γ)	${}^{A}_{Z}X + n \rightarrow {}^{A+1}_{Z}X + \gamma$
(n,p)	${}^{A}_{Z}X + n \rightarrow {}^{A}_{Z-1}Y + p$
(n,d)	${}^{A}_{Z}X + n \rightarrow {}^{A-1}_{Z-1}Y + d$
(n,t)	${}^{A}_{Z}X + n \rightarrow {}^{A-2}_{Z-1}Y + t$
$(n,{}^3He)$	${}^{A}_{Z}X + n \rightarrow {}^{A-2}_{Z-2}Y + {}^3He$
(n,α)	${}^{A}_{Z}X + n \rightarrow {}^{A-3}_{Z-2}Y + \alpha$
(n,f)	${}^{A}_{Z}X + n \rightarrow$ Fission Products + neutrons

$$N' = \mathbf{A}N \qquad (2)$$

$\boldsymbol{A}$ = transition matrix containing coefficients for decay and transmutation
N = nuclide concentration vector, *s.t.* $N = N_i$ for all i
N' = first derivative in time of nuclide concentration

The solution can be given in the form of an exponential as follows,

$$N = \exp(\mathbf{A}t)N(0) \qquad (3)$$

N(0) = initial nuclide concentration vector

The matrices produced in burnup problems exhibit one unique property which can be exploited to produce more accurate answers relatively quickly – the eigenvalues of the burnup matrix have been found to be bounded near the negative real axis Pusa (2011). Physically, this is a natural outcome of generating the burnup matrix; the diagonal elements represent the removal coefficients for a particular isotope and are always negative. For methods requiring solutions near the origin (the Taylor series expansion of the matrix exponential), this presents a mathematical hurdle.

CRAM takes advantage of this property and allows burnup matrices to be solved accurately without the removal of short-lived isotopes. For a full description on the derivation of CRAM, refer to Pusa and Leppanen (2010).

2.2. Linear chain solver

Burnup problems produce strictly structured and highly sparse matrices. Specifically, the resulting transition matrix containing all the coefficients corresponding to the set of ordinary differential equations governing the problem can be generated with recursive logic.

For the problem presented below,

$$N'(t) = \mathbf{A}N(t), \qquad (4)$$

where N is the vector of nuclide concentrations and A is the transition matrix holding all the relevant coefficients. The elements of A are defined as follows,

$$a_{ij} = \begin{cases} l_{ij}\lambda_j + (f_{ij}\sigma_j^f + nn_{ij}\sigma_j^{nn})\phi, & i \neq j \\ -(\lambda_i + \sigma_i\phi), & i = j \end{cases}, \qquad (5)$$

where, l_{ij} is the decay branching ratio of nuclide j to nuclide i, λ_j is the disintegration constant of nuclide j, f_{ij} is the yield fraction of the fission of nuclide j yielding nuclide i, σ_j^f is the fission cross section of nuclide j, σ_j^{nn} is the cross section for non-fission neutron reactions for nuclide j, nn_{ij} is the branching ratio of a non-fission neutron reaction with nuclide j yielding nuclide i, σ_j is the total cross section of nuclide j, and ϕ is the scalar neutron flux.