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BURNUP CODE AUTOMATION AND OPTIMIZATION - FUEL ASSEMBLY APPLICATION

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ABSTRACT

This work's main objective is to produce a computer program capable of performing precise burnup calculations considering a wide range of isotopes and transmutation processes. In this regard, the work parts from a preliminary burnup code version, coupled to VALKIN-FVM-Sn deterministic transport code developed at UPV. This version is analysed in detail and improved, increasing its capabilities and reducing its computation times. Several ODE methods are compared.

In this work, an initial fuel depletion program coupled with a transport code has been improved and depurated. Parting from satisfying results, the calculation process, execution time and performance have been enhanced.

1 INTRODUCTION

As computer capabilities and methods improve over the years, reactor physics programs are revised and enhanced following the increasing security concerns and demands. New computation capabilities allow the simulation of complex systems, and multiphysics simulations and analysis.

Burnup (or depletion) codes allow prediction of the isotope inventory evolution of systems exposed to a neutron flux and containing radioactive nuclides. In the case of nuclear reactors, where the systems are subjected to neutron fluxes induced by fission reactions and the isotope inventory contains a large number of nuclides, burnup codes must be fed with data

processed by transport codes. Transport codes provide problem-dependent cross-sections and fission yields, which are needed to obtain nuclide transmutation rates.

Transport codes are divided into stochastic and deterministic, depending on the approach used to solve the neutron transport equation. Both approaches present advantages and disadvantages. Most of the current developments in depletion codes associated with stochastic transport codes, namely ACAB [1], ALEPH-2 [2], SERPENT [3], FISPACT-II [4], or ONIX [5]. However, burnup codes based on deterministic transport solvers are widely used in research and industry, for example, CASMO [6] and SCALE [7].

The present work shares the advances in developing a brand-new burnup code coupled with VALKIN-FVM-Sn deterministic transport solver [8]. The depletion code is intended to be part of a reactor physics program with Multiphysics capabilities. The resulting program will have advantages such as the VALKIN-FVM-Sn 2D and 3D computation capabilities and its ability to deal with complex geometries using unstructured meshes, which overcome one of the major deterministic solver's drawbacks.

The starting point is a burnup code developed in MATLAB© and coupled to VALKIN-FVM-Sn. This code has been translated and tested in FORTRAN. Two solvers have been evaluated. The result is a burnup code coupled to a deterministic transport solver capable of performing depletion calculations using a detailed burnup chain.

2 THE BURNUP PROBLEM

Materials inside a nuclear reactor can experience an isotope evolution, mainly due to two transmutations mechanisms: neutron-induced reactions and decay processes. Nuclear fuel is the element that presents the most complex scenario in terms of isotope change as it contains the fissile species. Fissions inside nuclear fuel mainly determines the thermal output during operation and produces fission products, leading to thousands of different nuclides. The change in fuel isotope inventory leads to an important change in the element reactivity during the burnup.

Nuclide evolution during time is mathematically calculated as in Eq. (1), known as Bateman equation [9] or burnup equation, a first order linear Ordinary Differential Equation (ODE).

$$\frac{dN_i}{dt} = \sum_{j(j\neq i)}(b_{i,j}\lambda_j + \sum_k \gamma_{i,j,k}\sigma_{j,k}\phi)N_j - (\lambda_i + \sigma_{rem,i}\phi)N_i \quad (1)$$

In Eq. (1) , N_i is the nuclide i atom density; $b_{i,j}$ is the branching ratio from nuclide j to i; λ_j is the decay constant of nuclide j; ϕ is the space- and energy- average neutron flux; $\sigma_{j,k}$ is the microscopic cross-section of reaction k for nuclide j; $\sigma_{rem,i} = \sum_k \sigma_{i,k}$, is the removal cross-section of nuclide i, obtained by adding all possible neutron-induced reactions, k, that nuclide i can experience; and $\gamma_{i,j,k}$ is the production yield of nuclide i due to the reaction k occurred in nuclide j, including the non-fission and fission events.

Nuclides are organized into groups depending on the existence or lack of one of the terms from Eq. (1). In this work two groups are considered: fissionable nuclides (present fission cross section and lack yield contribution from fission) and fission products (lack fission cross section and present yield contribution from fission).

In a material containing several nuclides and under a neutron flux, its isotopic evolution is defined as a set of coupled Batman's equations, which leads to a first order (ODE) system,

that can be expressed in matrix notation as in Eq. (2). Neutron-induced coefficients and flux depend on the concentrations. In order to be able to solve the ODE system, cross-sections, flux, and other problem dependent parameters are supposed constant for periods of time denoted as *Depletion Steps* (n). Then, the concentrations can be obtained for each *Depletion Step*.

$$\frac{d\vec{N}}{dt} = A\vec{N}(t) = (A_{\sigma,n}\phi_n + A_\lambda)\vec{N}(t) \tag{2}$$

A is the *Transition Matrix*, which contains the system coefficients (transition rates); $\vec{N}(t)$ is the concentration vector; $A_{\sigma,n}$ is the *Transition Matrix* part containing neutron-induced transitions for the step n; ϕ_n is the space and energy averaged neutron flux for step n; and A_λ is the *Transition Matrix* part holding decay transitions.

Nuclides, and possible transitions between them form *Burnup-chains*, which can be represented as in Figure 1. Nowadays, computational capabilities allow to consider extensive *burnup-chains* considering thousands of nuclides and dozens of transitions.

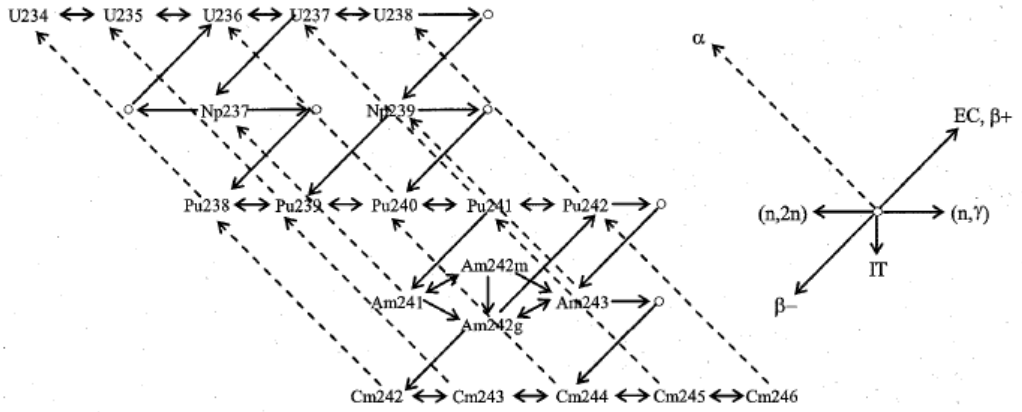

Figure 1: SRAC's standard chain model for actinides (ucm6~) [10]

Solving Eq. 2 is a well-known problem and widely studied, for example in [11], [12] or [13].

3 METHODOLOGY

In order to create an effective and accurate depletion program linked to VALKIN-FVM-Sn, a preliminary version was first developed in MATLAB©, as it presents a comfortable environment to evaluate the whole calculation process and results. Once the preliminary version has been completed, a FORTRAN version making use of more sophisticated and powerful ODE solvers is created.

The code developed and libraries used were created considering several codes as example, but the main reference was chosen to be SCALE, version 6.2.4 [7].

3.1 Burnup-chain

An extensive *burnup-chain* has been used to perform the depletion calculations, 1327 nuclides are considered, 1151 fission products and 176 actinides. In regard of transitions between nuclides, 21 neutron-induced reactions and 11 decay mechanisms are considered, shown in Table 1 and Table 2 .

Table 1: Neutron reactions

Neutron-induced reactions		
Number	MT number	Reaction
1	16	$(n, 2n)$
2	17	$(n, 3n)$
3	18	$(n, fission)$
4	22	$(n, n\alpha)$
5	24	$(n, 2n\alpha)$
6	28	(n, np)
7	29	$(n, n2\alpha)$
8	32	(n, nd)
9	33	(n, nt)
10	34	$(n, n\ ^3He)$
11	37	$(n, 4n)$
12	41	$(n, 2np)$
13	102	(n, γ)
14	103	(n, p)
15	104	(n, d)
16	105	$(n,\ ^3He)$
17	106	(n, t)
18	107	(n, α)
19	108	$(n, 2\alpha)$
20	111	$(n, 2p)$
21	112	$(n, p\alpha)$

Table 2: Decay processes

Decay mechanisms	
Number	Decay
1	$\beta^-[m0]$
2	$\beta^-[m0] + \alpha$
3	$\beta^-[m1]$
4	$\beta^-[m0]$
5	$\beta^-[m0] + \alpha$
6	$\beta^-[m0] + n$
7	$\beta^+[m0]$
8	$\beta^+[m1]$
9	$\alpha\ [m0]$
10	$\alpha\ [m1]$
11	m

3.2 Program workflow, coupling, and data libraries

For each depletion step the burnup code needs to be fed with information depicted in Eq. 2. Neutron-induced *Transition Matrix* and integral flux must be computed using the flux spectrum resulting from a transport calculation. In order to perform transport calculations, self-shielded cross-sections were obtained with SCALE's ***xsproc*** module for each depletion step.

VALKIN-FVM-Sn is coupled to a burnup code to create the problem-dependent depletion data. The program workflow is as follows: for each depletion step the transport code is executed, then the material flux spectrum is obtained. With the flux, the problem-dependent depletion parameters are obtained, and finally, the burnup code perform the depletion calculation. With the new concentration the process is to be re-started again for each depletion step.

The problem-dependent parameters to be computed for depletion step are:

1. Collapsed one-group cross sections.
2. Time- and space- integral flux.
3. Interpolated yield.

The problem-dependent parameters are created from problem-independent libraries:

- Neutron library. Based on the JEFF-3.0/A [14].
- Fission yield library. Based on the ENDF/B-VII.0 [15]
- Energy released library. Based on the ENDF/B-VII.0

Decay *Transition Matrix* is constant, and its values comes from the ENDF/B-VII.I [16].

3.3 ODE solvers

In this work a MATLAB© version of the depletion code was translated to modern FORTRAN. Two solvers were tested, **ode15s** [17] has been used in MATLAB© as it is recommended for stiff problems, and **lsode** [18] has been used in FORTRAN. In the **lsode** case, it was used because of its capabilities and easy implementation, it has also been used for depletion problems in codes such as FISPACT-II [4].

3.4 Reference model

To verify the developed program three depletion calculation were performed, the results obtained by FORTRAN and MATLAB© were compared by a reference calculation. The reference results were obtained from SCALE 6.2.4. A single fuel pin was modelled to assess the programs performance, it corresponds to the TMI-1 PWR unit cell from UAM benchmark [19], it is defined in Table 3 and Figure 2.

Table 3: Pin model information

Parameters	Value
Unit cell pitch, [mm]	14.427
Fuel pellet diameter, [mm]	9.391
Fuel pellet material	UO_2
Fuel density, [g/cm^3]	10.283
Fuel enrichment, w/o	4.85
Cladding outside diameter, [mm]	10.928
Cladding thickness, [mm]	0.673
Cladding material Cladding density, [g/cm^3]	Zircaloy – 4 6.55
Gap material	He
Moderator material	H_2O
Fuel temperature, [K]	900
Cladding temperature, [K]	600
Moderator (coolant) temperature, [K]	562
Moderator (coolant) density, [kg/m^3]	748.4
Power density, [MW/MTHM]	25

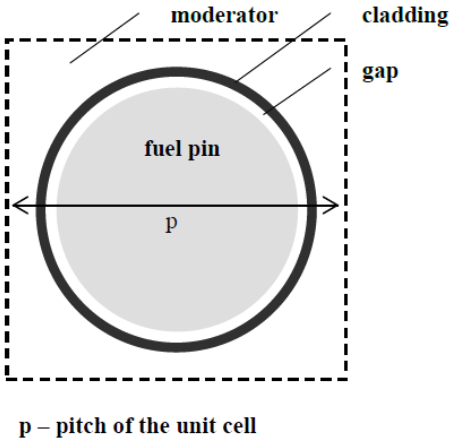

Figure 2: Pin model geometry

Burnup was performed for 365 days with 25 MW/MTHW power density, using 16 uniformly distributed depletion steps.

4 RESULTS

This work's main objective is to translate the coupled burnup program to FORTRAN. With this, it is intended to reduce calculation times, and to use a more powerful ODE solver. Calculations were performed using a workstation with an Intel Core i7-4790 3.6GHz CPU. VALKIN-FVM-Sn is also written in FORTRAN, this work will help further integration between programs and additional improvements. Furthermore, additional modules are to be develop in FORTRAN, for example, a cross section processing module.

From all over the processes and calculations to be performed by the program, there are two tasks that are more time consuming both in MATLAB© and FORTRAN: charging data libraries and solving the ODE systems. Libraries charging is independent from the case study as the libraries are always constant. By using FORTRAN, the time invested in this task have been reduced 27%, from 3.4 seconds to 2.5 seconds in average.

As can be seen in Table 4, results at the end of the depletion are the same for MATLAB© and FORTRAN programs. Both present low relative errors compare to the reference. Nevertheless, the time required to solve each depletion step is considerably lower using **lsode**, as shared in Table 5, over 90% less time is required by **lsode**.

Table 4: Nuclide concentrations at the end of the depletion

	SCALE	MATLAB (ode15s)		FORTRAN (lsode)	
NUCLIDE	Concentration (atm/bcm)	Concentration (atm/bcm)	Rel. Dif. (%)	Concentration (atm/bcm)	Rel. Dif. (%)
Se-79	1.006E-07	1.026E-07	-1.904E+00	1.026E-07	-1.904E+00
Kr-83	1.084E-06	1.106E-06	-2.022E+00	1.106E-06	-2.022E+00
Sr-90	1.165E-05	1.190E-05	-2.139E+00	1.190E-05	-2.139E+00
Y-91	2.654E-06	2.730E-06	-2.859E+00	2.730E-06	-2.859E+00
Mo-95	8.634E-06	8.791E-06	-1.827E+00	8.791E-06	-1.827E+00
Tc-99	8.634E-06	8.791E-06	-1.827E+00	8.791E-06	-1.827E+00
Ag-109	3.934E-07	3.958E-07	-6.213E-01	3.958E-07	-6.213E-01
Sn-126	1.773E-07	1.794E-07	-1.133E+00	1.794E-07	-1.133E+00
I-129	1.431E-06	1.453E-06	-1.513E+00	1.453E-06	-1.513E+00
Xe-136	2.228E-05	2.278E-05	-2.223E+00	2.278E-05	-2.223E+00
Cs-133	1.419E-05	1.447E-05	-1.968E+00	1.447E-05	-1.968E+00
Ce-142	1.272E-05	1.297E-05	-2.007E+00	1.297E-05	-2.007E+00
Pr-144	3.284E-10	3.354E-10	-2.133E+00	3.354E-10	-2.133E+00
Nd-144	4.633E-06	4.727E-06	-2.018E+00	4.727E-06	-2.018E+00
Sm-147	4.810E-07	4.903E-07	-1.946E+00	4.903E-07	-1.946E+00
Gd-155	6.375E-10	6.285E-10	1.411E+00	6.285E-10	1.411E+00
U-235	8.909E-04	8.866E-04	4.913E-01	8.866E-04	4.913E-01
U-238	2.169E-02	2.169E-02	-4.608E-03	2.169E-02	-4.608E-03
Np-237	1.544E-06	1.510E-06	2.200E+00	1.510E-06	2.200E+00
Pu-239	7.595E-05	7.501E-05	1.241E+00	7.501E-05	1.241E+00
Am-241	3.699E-08	3.694E-08	1.372E-01	3.694E-08	1.373E-01

5 CONCLUSIONS

At the end of this work a FORTRAN burnup code coupled to VALKIN-FVM-Sn transport code has been developed. The resulting program can perform depletion calculations using a detailed burnup chain with a large number of nuclides and transitions. It uses the **lsode** solver to compute the ODE systems with a reasonable time consuming.

Table 5: Calculation time required for each depletion step

	Calculation times (s)		
Depletion step	ode15s	lsode	Time reduction (%)
1	47.78258	3.121341	93.467616
2	26.23782	2.869217	89.064577
3	22.36579	2.10504	90.588129
4	21.80142	1.725517	92.085298
5	17.50912	1.776411	89.854365
6	18.26346	1.789384	90.202382
7	22.40954	1.839636	91.790838
8	19.42885	1.879585	90.325803
9	20.15101	1.871584	90.712208
10	23.08222	1.907503	91.736051
11	22.38153	1.878595	91.606491
12	20.23785	1.902531	90.599147
13	19.14423	1.883856	90.159668
14	22.7675	1.897394	91.666216
15	22.25339	1.948792	91.24272
16	22.68101	1.905254	91.599781

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