MEDEAC: Matrix Exponential based isotope DEpletion and Analysis Code

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1. Introduction

ORIGEN code [1] has been widely used to estimate the radioactive material inventory in the core or in the spent fuel repository. KAERI also has been used this code for various core design area. Recently, KAERI has been conducting the SMART-PPE project with the Saudi Arabia, and transmitting the design technology to the Saudi engineer. Undergoing the project in early time, the Saudi engineer did not take the license for the DOORS codes such as ORIGEN and MCNP. Therefore, KAERI decided to develop an alternative code to the DOORS codes. Currently, Saudi engineer took the license for the DOORS code package.

MEDEAC is developed for an alternative code to ORIGEN by improving the capability of the DeCBURN program [2] which is originally developed for DeCART [3] depletion calculation by using the Krylov subspace method. This paper first describes the code requirements for MEDEAC, and then explains the main method of the Krylov subspace method and the code models briefly. Finally, the calculation results are examined by comparing the ORIGEN code and the fine time step results of MEDEAC.

2. Methods and Results

In this section the code requirement, the key solution method of Krylov subspace method, some models, code structure and the calculation results are described.

2.1 Functional Requirements

In developing MEDEAC, the ORIGEN code is used as a role code. Therefore, the code requirements are all established from the ORIGEN functions as:

- Depletion Calculation Capability with Constant Power or Flux Condition
- Isotope Composition in mol
- Total Radioactivity in Ci
- Alpha Radioactivity in Ci
- Total Power in W
- Decay Heat in W
- Decay induced Gamma Power in W
- Air volume in m^3 to meet RCG (Radioactivity Concentration Guide) Inhalation Requirement
- Water volume in m^3 to meet RCG Ingestion Requirement
- Water volume in m^3 to meet Chemical Ingestion Requirement
- (α,n) Neutron Source in #/sec
- Spontaneous Neutron Source in #/sec
- Photon Emission Rate in #/sec

2.2 Krylov Subspace Method

To solve the burnup equation, the Krylov subspace method expands the solution vector of $\mathbf{X}(t)$ by the Krylov subspace of dimension m as:

$$K_m\{\mathbf{A}t,\ \mathbf{X}(0)\} = \mathbf{span}\{\mathbf{X}(0), (\mathbf{A}t)^1\mathbf{X}(0), \dots, (\mathbf{A}t)^{m-1}\mathbf{X}(0)\} \quad (1)$$

and generates the orthonormal basis by using Arnoldi procedure.

The relation between the original burnup matrix and the orthogonal matrix can be written as:

$$\mathbf{H}_m = \mathbf{V}_m^T(\mathbf{A}t)\mathbf{V}_m \quad (2)$$

where

$\mathbf{V}_m = [\mathbf{v}_1 \quad \cdots \quad \mathbf{v}_m] \in \mathbf{R}^{n\times m}$
$\mathbf{H}_m \in \mathbf{R}^{m\times m}$: Hessenberg Matrix
$\mathbf{v_i}$: orthonormal vector
m: order of Krylov subspace

Using the orthonormal basis vectors, the solution is approximated as:

$$\tilde{\mathbf{X}}(t) = \mathbf{V}_m\mathbf{y}_{approx} = \boldsymbol{\beta}\mathbf{V}_m\,\mathbf{exp}(\mathbf{H}_m t)\,\mathbf{e}_1 \quad (3)$$

where

$\tilde{\mathbf{X}}(t)$: Approximate solution of $\mathbf{X}(t)$
$\mathbf{X}(0) = \boldsymbol{\beta}\mathbf{v}_1 = \boldsymbol{\beta}\mathbf{V}_m\mathbf{e}_1$

The followings are some features of MEDEAC when applying the Krylov subspace method to matrix exponential.

- Matrix condensation is performed to remove the short lived isotopes with the criteria of 1,000.0.
- The Krylov subspace method is applied to the condensed matrix with the order of 100. When solving the matrix exponential, the scaling and squaring technique is used. The scaling technique reduces the maximum element of matrix to less than 0.01. The solution of scaled matrix exponential is approximated as:
$$\exp\left(\tilde{\mathbf{H}}_m t\right) \approx \mathbf{I} + \tilde{\mathbf{H}}_m t$$
- For the short lived isotopes, the equilibrium condition is applied. The solution is obtained by

the iterative algorithm by sweeping all short lived isotopes a few times.
- Predictor-Corrector scheme is used for the constant power condition, where the flux is varied with the time.
- Once-through depletion scheme is used for the constant flux or zero power conditions.

2.3 Models

This Section describes the calculation models to meet the requirements of MEDEAC. In the current status, most models are obtained from the ORIGEN code.

The fission energy (κ) released from a fission is approximated as:

$$\kappa(Mev/fission) = a_1\left(Z^2 A^{0.5}\right) + a_2 \quad (4)$$

where a_1=1.29927x10-3 and a_2=33.12. The above model is known to predict with a maximum error of 1 % for nuclides between ^{232}Th and ^{242}Pu.

The other models are summarized as:

- Total 42 spontaneous fission isotopes are treated in the code. The neutron yield data are fixed in the code.
- Total 32 fission isotopes are treated in the code. The neutron yield data are fixed in the code.
- Total 8 fission product yield isotopes are treated. The isotopes are ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu, ^{245}Cm and ^{252}Cf, and fixed in the code. The yield data are given through the library.
- Total 18 gamma energy groups are treated in the code. The energy group structure are fixed in the code and the gamma yield data are given through the library.
- Total 8 (α,n) isotopes are treated. The (α,n) isotopes are ^{235}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Am, ^{242}Cm and ^{244}Cm, and fixed in the code with the neutron yield data.
- The chemical toxicity in g/m^3 for all elements are treated. The toxicity data are fixed in the code.
- To calculate the volume to meet the RCG requirement, the hazard data in m^3/Ci are given through the library.
- Total 8 decay types are treated as the ORIGEN code. The decay constant and fraction data are given through the library.
- Total 8 reaction types are treated as the ORIGEN code. The one group cross sections are given through the library.

2.4 Code Structure

Fig. 1 shows the code structures for MEDEAC and ORIGEN. ORIGEN requires three types of libraries which includes one cross section library, one decay data library, and one photon library. MEDEAC requires one library because it includes all data of three ORIGEN library. MEDEAC generates two output files, a normal output and a summary output files. The contents of the summary output file are as follows:

(1) EDIT 1: Overall results such as burnup, power, flux, k-inf, decay heat, decay gamma power, radioactivity, air and water volumes for RCG requirements, chemical toxicity.
(2) EDIT 2: Composition changes in mol for some important isotopes
(3) EDIT 3: Composition changes in gram for some important isotopes
(4) EDIT 4: Group-wise gamma amounts
(5) EDIT 5: Group-wise gamma power
(6) EDIT 6: Neutron sources from spontaneous fission, (α,n), neutron induced fission

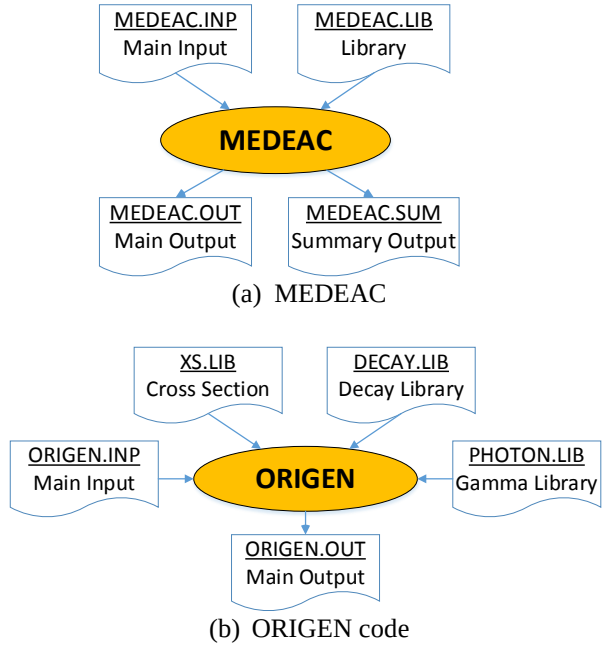

Fig. 1. Code structures for MEDEAC and ORIGEN

2.5 Examination and Results

MEDEAC is applied to 4.0 w/o UO2 fuel pin. The followings are the summary of the problem:

- Total mass of UO2: 5 gram
- Depletion Condition: Constant flux of 1.0E14
- Depletion to 100 day
- Solution Comparison at 100 day

For the comparison, the following three results are obtained.

- REF: the reference solution obtained by MEDEAC with the fine time step size of 0.002 day. This condition eliminates the short-lived isotopes, and the result for all isotopes is obtained by matrix exponential method.
- ORI: ORIGEN solution obtained with the time step size of 1.0 day.
- MED: MEDEAC solution at the time points of 5, 15, 30, 60, 90, 100 day. The time points are also used for depletion steps. This is a general condition for isotope depletion.

Fig. 2 shows how to generate the MEDEAC library. Program LIBCONV is used to convert the ORIGEN library to MEDEAC library or vise versa. MEDEAC library includes all information of ORIGEN libraries.

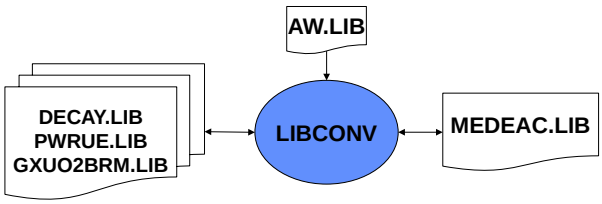

Fig. 2. MEDEAC library generation

Table I, II, III show the error in atomic inventory at 100 day for the activation product, actinides, and fission products, respectively. MED predicts almost the same atomic inventories with REF showing a trivial error of about 1.0% for the element with very low inventory. ORIGEN also agrees well with the REF solutions, but shows larger errors than MED even though it uses the less time step size. In additional comparison with 1.0 depletion size, MEDEAC eliminated even the trivial error of about 1.0% of MED. This result means that MEDEAC can estimate the isotope inventory very well with the normal depletion step size of 30 days.

Table IV shows the summary results at 100 day. MEDEAC shows almost the same results with the ORIGEN code. This result means that MEDEAC equips most computational functions of the ORIGEN code, and estimates the radioactive material data very well.

Table I: Activation Product Inventory (mol) at 100 day

Z	REF[1)]	Err, %	
		MED[2)]	ORI[3)]
H	1.30E-10	0.00	-0.31
He	8.54E-08	0.00	0.00
Li	4.54E-23	0.00	-4.87
Be	2.15E-14	0.00	0.00
B	2.56E-20	0.00	-0.04
C	8.54E-08	0.00	0.00
N	2.20E-11	0.00	0.00
O	3.71E-02	0.00	0.00
F	1.80E-12	0.00	0.06
Ne	7.30E-19	0.00	0.07

1) MEDEAC solution with 0.002 day depletion size
2) MEDEAC solution with 5, 15, 30, 60, 90, 100 depletion time
3) ORIGEN solution with 1.0 day depletion size

Table II: Actinide Inventory (mol) at 100 day

Z	REF	Err, %	
		MED	ORI
He	5.05E-11	0.00	0.04
Tl	3.82E-24	0.00	2.23
Pb	8.03E-20	0.01	3.49
Bi	2.07E-22	0.00	1.36
Po	1.39E-26	-0.93	-37.95
Rn	3.21E-24	0.00	-0.06
Fr	1.47E-26	-1.43	-2.52
Ra	1.90E-20	0.00	0.00
Ac	5.44E-19	0.00	0.00
Th	2.74E-13	0.00	0.00
Pa	1.92E-13	0.00	0.00
U	1.85E-02	0.00	0.00
Np	5.30E-07	0.00	-0.26
Pu	1.22E-05	0.00	0.00
Am	5.46E-11	-0.02	0.09
Cm	5.68E-13	0.00	0.11

Table III: Fission Product Inventory (mol) at 100 day

Z	REF	Err, %		Z	REF	Err, %	
		MED	ORI			MED	ORI
H	3.04E-09	0.00	0.03	Ag	3.07E-08	0.00	0.03
Li	1.29E-11	0.00	0.00	Cd	6.04E-08	0.00	0.02
Be	2.73E-12	0.00	0.04	In	9.36E-09	0.00	0.03
C	3.38E-13	0.00	0.00	Sn	9.64E-08	0.00	1.13
Co	3.05E-20	0.00	0.00	Sb	4.13E-08	0.00	-0.02
Ni	1.16E-17	0.00	0.09	Te	6.08E-07	0.00	0.02
Cu	1.09E-16	0.00	0.00	I	3.56E-07	0.00	2.95
Zn	1.49E-11	0.00	0.00	Xe	6.27E-06	0.00	0.29
Ga	7.03E-13	0.00	0.00	Cs	4.12E-06	0.00	0.10
Ge	1.67E-09	0.00	0.00	Ba	2.04E-06	0.00	0.00
As	5.62E-10	0.00	0.02	La	1.70E-06	0.00	0.00
Se	1.41E-07	0.00	0.00	Ce	4.65E-06	0.00	0.04
Br	5.57E-08	0.02	0.02	Pr	1.18E-06	0.00	0.08
Kr	9.78E-07	0.00	0.03	Nd	3.83E-06	0.00	0.03
Rb	9.00E-07	0.01	0.02	Pm	4.82E-07	0.00	0.00
Sr	3.01E-06	0.00	0.53	Sm	5.23E-07	0.00	0.23
Y	1.42E-06	0.00	1.06	Eu	6.10E-08	0.00	0.02
Zr	7.96E-06	0.00	0.16	Gd	1.04E-08	0.00	0.00
Nb	3.50E-07	0.00	0.03	Tb	7.01E-10	0.01	0.07
Mo	5.00E-06	0.00	0.84	Dy	2.66E-10	0.04	0.04

Tc	1.49E-06	0.00	0.07	Ho	1.24E-11	0.00	0.08
Ru	3.60E-06	0.00	0.03	Er	9.35E-12	0.00	0.01
Rh	4.61E-07	0.00	0.09	Tm	2.75E-17	0.00	0.00
Pb	4.98E-07	0.00	0.08	Yb	2.18E-20	0.00	-0.05

Table IV: Summary Results at 100 day

Parameter	MED	ORI
Power, W	5.87E+01	5.88E+01
Decay Heat, W	3.70E+00	3.70E+00
Decay Gamma Power, W	1.02E+00	1.02E+00
Radioactivity, Ci	3.27E+02	3.28E+02
Alpha Activity, Ci	1.98E-04	1.98E-04
Air Volume for RCG, m^3	1.22E+11	1.21E+11
Water Volume for RCG, m^3	5.75E+08	5.75E+08
Water Volume for Chemical, m^3	1.26E+01	1.26E+01
(α,n) Neutrons	1.45E-01	1.45E-01

3. Conclusions

MEDEAC is developed in this paper for an alternative code to the ORIGEN code by improving the DeCBURN program, and the solution is examined by comparing with the MEDEAC solution with fine depletion step size and the ORIGEN solution. The ORIGEN code is used as a role code, so MEDEAC is designed to generate most results of the ORIGEN code. The results show that MEDEAC estimates the isotope inventory comparably and the radioactive data very closely with the ORIGEN code. These results mean that MEDEAC works soundly and can be used as an alternative code to the ORIGEN code.

In the future, update for the MEDEAC library and the solution method will be performed.

REFERENCES

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