MEDEAC: Matrix Exponential based isotope DEpletion and Analysis Code

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Contents

Sungmin Kim et al, "Comparison of MEDEAC and ORIGEN in Fuel Assembly Depletion Calculation," '2017 KNS Autumn Meeting, Gyeongju, Korea, 2017

Introduction

- **ORIGEN code**
  - **Developed by ORNL**
  - **Used to Estimate the Radioactive Material Inventory in Core or in Spent Fuel Repository**
  - **Used for SMART Radioactive Inventory Source and Decay Heat**
- **HCB (Human Capability Buildup) for Saudi Engineer**
  - **CRT Basic and Technical, OJT Basic and In-depth, OJP**
- **Code License Limit for Saudi Engineer**
  - **Site License**
  - **MCNP -> McCARD**
  - **DORT -> AETIUS**
  - **ORIGEN -> MEDEAC**
- **Currently, Saudi Engineer obtained License for MCNP and ORIGEN**

Code Requirements

- **Function of the ORIGEN Code**
  - **Depletion with Step Power or Flux Variation**
  - **Isotope Composition in mol**
  - **Flux or Thermal Power in W**
  - **Decay Heat in W**
  - **Decay Induced Gamma Power in W**
  - **Radioactivity in Ci**
  - **Alpha (α) Radioactivity in Ci**
  - **m^3 air to meet RCG (Radioactivity Concentration Guide) Inhalation**
  - **m^3 water to meet RCG Ingestion Requirement**
  - **m^3 water to meet Chemical Ingestion Requirement**
  - **(α,n) Neutron Source in /sec**
  - **Spontaneous Neutron Source in /sec**
  - **Photon Emission Rate in /sec**
- **ORIGEN is Role Code for MEDEAC**

Models

- **Fission Energy (κ) model**

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

$$a_1 = 1.29927 \times 10^{-3}$$

$$a_2 = 33.12$$

  - **Predicts with a maximum error of 1 % for nuclides between ^{232}Th and ^{242}Pu**

- **Data fixed in the Code**
  - **Total 42 Spontaneous Fission Isotopes and their Neutron Yields**
  - **Total 32 Fission Isotopes and their Neutron Yields**
  - **18 Gamma Energy Group Structure**
  - **Neutron Yield from (α, n) reactions**
    - **8 Isotopes: ^{235}U, ^{238}U, ^{238}Pu , ^{239}Pu, ^{240}Pu , ^{241}Am , ^{242}Cm , ^{244}Cm**
  - **Atomic Chemical Toxicity in g/m^3 water**
  - **Fission Product Yield Isotope**
    - **8 Isotopes: ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu , ^{245}Cm , ^{252}Cf**

Models

◆ Data in the Library

- Atomic Weight
- Atomic Abundance
- Decay Constant
- Decay Heat Recoverable (Q)
- RCG for Inhalation in Ci/m^3 air (10CFR20 App. B Table 2)
- RCG for Ingestion in Ci/m^3 water (10CFR20 App. B Table 2)
- Decay Fraction Data
- Neutron Cross Section
- Gamma Yield Data for 18 Gamma Groups
- Fission Product Yield Data for 8 Isotopes

Chain Buildup

◆ Decay Chain

Order	Decay Type	Final Isotope
1	β^- decay to exited state	${}_{Z+1}^{A}X^m$
2	β^+ or electron capture	${}_{Z-1}^{A}X$
3	β^+ or electron capture to exited state	${}_{Z-1}^{A}X^m$
4	alpha decay	${}_{Z-2}^{A-4}X+\alpha$
5	Isomeric transition	${}_{Z}^{A}X^m \rightarrow {}_{Z}^{A}X$
6	Spontaneous Fission	
7	$(\beta^- + n)$ decay	${}_{Z+1}^{A-1}X + n$
Remaining	β^- decay to stable state	${}_{Z+1}^{A}X$

Chain Buildup

◆ Reaction Chain

Order		Reaction Type	Final Isotope
1		(n,γ)	${}^{A+1}_{Z}X$
2		$(n,2n)$	${}^{A-1}_{Z}X$
3	Activation & F.P	(n,α)	${}^{A-3}_{Z-2}X$
	Actinide	$(n,3n)$	${}^{A-2}_{Z}X$
4	Activation & F.P	(n,p)	${}^{A}_{Z-1}X$
	Actinide	Fission	
5		(n,γ')	${}^{A-1}_{Z}X^{m}$
6		$(n,2n')$	${}^{A+1}_{Z}X^{m}$

Krylov Subspace Method

- **Krylov subspace method for Matrix exponential**
  - $\mathbf{X}(t)$ **approximation by the Krylov subspace of dimension m as:**

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

  - **Orthonormal basis of the Krylov subspace by using Arnoldi procedure**
- **Features of Arnoldi procedure**
  - $\mathbf{H}_m = \mathbf{V}_m^T(\mathbf{A}\boldsymbol{t})\mathbf{V}_m$
    - $\mathbf{V}_m = [\mathbf{v}_1 \quad \cdots \quad \mathbf{v}_m] \in \mathbf{R}^{n\times m}$, $\mathbf{H}_m \in \mathbf{R}^{m\times m}$: **Hessenberg Matrix**
    - $\mathbf{V}_m^T\mathbf{V}_m = \mathbf{I}$, $\mathbf{V}_m^T\mathbf{v}_{m+1} = \mathbf{0}$
- **Approximate solution using Krylov subspace**

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

where

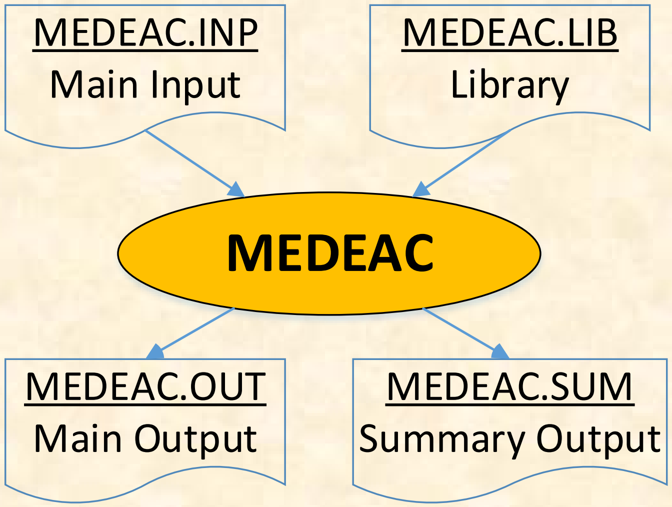
$\widetilde{\mathbf{X}}(t)$: **Approximate solution of** $\mathbf{X}(t)$

$\mathbf{X}(0) = \beta\mathbf{v}_1 = \beta\mathbf{V}_m\mathbf{e}_1$

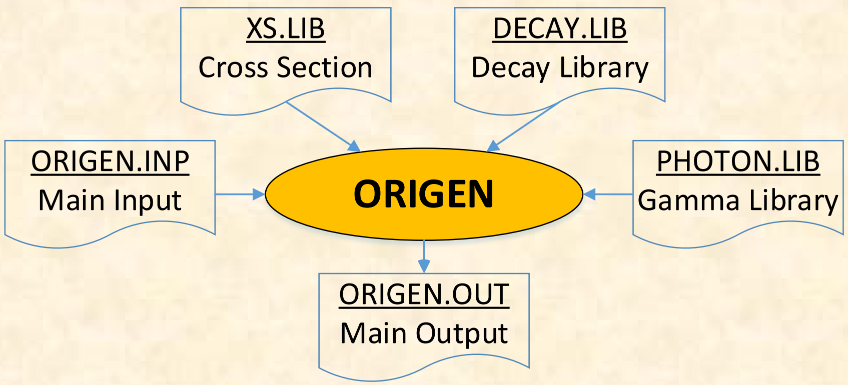
Feature of Solver

- **Matrix Condensation by Removing the Short Lived Isotope**
- **Equilibrium Condition for Short Lived Isotopes**
  - $\frac{d}{dt}N_i \sim 0$
  - **Apply Iterative Algorithm**
  - **Criteria for Short Lived Isotopes: $a_{ii} > 1,000$**
- **Matrix Exponential Solution for Long Lived Isotopes**
  - **Krylov Subspace Method with order 100**
  - **Scaling and Squaring Technique**
  - **Scaling to $\|\mathrm{H}_m t\|_1 < 0.01 \rightarrow \exp\left(\tilde{H}_m t\right) \approx \mathbf{I} + \tilde{H}_m t$**
- **Predictor-Corrector Scheme for Constant Power Condition**
- **Once-Through Depletion Scheme for Constant Flux or Zero Power Condition**

Code Structure



MEDEAC Code Structure



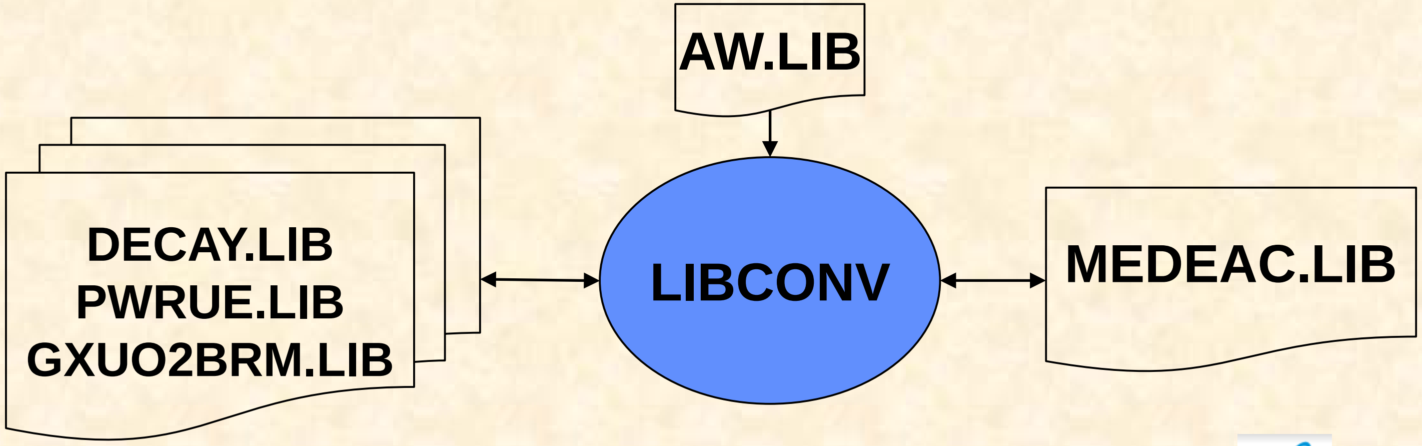
ORIGEN Code Structure

◆ Contents of Summary Output

- **Edit 1: Overall Results (Bu, Pow, ϕ, k-inf, Decay Heat, Pow-γ, Ci, RCG in air, RCG in water, Chemical Toxicity in water)**
- **Edit 2: Composition Change in mol for important Isotopes**
- **Edit 3: Composition Change in gram for important Isotopes**
- **Edit 4: Group-wise Gamma Amounts**
- **Edit5: Group-wise Photon Energy**
- **Edit 6: Neutron Sources ((α, n), Spontaneous Fission, Fission, Secondary Source)**

Examination

- **Problem**
  - **Material: 5 g of UO_2 fuel with 4.0 w/o**
  - **Depletion Condition: Constant Flux of 1.0×10^{14}**
  - **Depletion to 100 EFPD**
- **Comparison**
  - **MED: Solution with Time Points of 0, 5, 15, 30, 60, 90, 100 day**
  - **REF: $\Delta t = 0.002$ day using MEDEAC, ORI: $\Delta t = 1.0$ day**
  - **Isotope Number Density, and Summary Result at 100 EFPD**
- **Library Generation**



Atomic Inventory (mol) at 100 Day

Activation Product

Z	REF	Err, %	
		MED	ORI
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

Actinides

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

Fission Product Inventory (mol) at 100 Day

Z	REF	Err, %		Z	REF	Err, %		Z	REF	Err, %	
		MED	ORI			MED	ORI			MED	ORI
H	3.04E-09	0.00	0.03	Y	1.42E-06	0.00	1.06	Cs	4.12E-06	0.00	0.10
Li	1.29E-11	0.00	0.00	Zr	7.96E-06	0.00	0.16	Ba	2.04E-06	0.00	0.00
Be	2.73E-12	0.00	0.04	Nb	3.50E-07	0.00	0.03	La	1.70E-06	0.00	0.00
C	3.38E-13	0.00	0.00	Mo	5.00E-06	0.00	0.84	Ce	4.65E-06	0.00	0.04
Co	3.05E-20	0.00	0.00	Tc	1.49E-06	0.00	0.07	Pr	1.18E-06	0.00	0.08
Ni	1.16E-17	0.00	0.09	Ru	3.60E-06	0.00	0.03	Nd	3.83E-06	0.00	0.03
Cu	1.09E-16	0.00	0.00	Rh	4.61E-07	0.00	0.09	Pm	4.82E-07	0.00	0.00
Zn	1.49E-11	0.00	0.00	Pb	4.98E-07	0.00	0.08	Sm	5.23E-07	0.00	0.23
Ga	7.03E-13	0.00	0.00	Ag	3.07E-08	0.00	0.03	Eu	6.10E-08	0.00	0.02
Ge	1.67E-09	0.00	0.00	Cd	6.04E-08	0.00	0.02	Gd	1.04E-08	0.00	0.00
As	5.62E-10	0.00	0.02	In	9.36E-09	0.00	0.03	Tb	7.01E-10	0.01	0.07
Se	1.41E-07	0.00	0.00	Sn	9.64E-08	0.00	1.13	Dy	2.66E-10	0.04	0.04
Br	5.57E-08	0.02	0.02	Sb	4.13E-08	0.00	-0.02	Ho	1.24E-11	0.00	0.08
Kr	9.78E-07	0.00	0.03	Te	6.08E-07	0.00	0.02	Er	9.35E-12	0.00	0.01
Rb	9.00E-07	0.01	0.02	I	3.56E-07	0.00	2.95	Tm	2.75E-17	0.00	0.00
Sr	3.01E-06	0.00	0.53	Xe	6.27E-06	0.00	0.29	Yb	2.18E-20	0.00	-0.05

Summary Results at 100 Day

Parameter	MEDEAC	ORIGEN
Power, W	5.87E+01	5.88E+01
Decay Heat, W	3.70E+00	3.70E+00
Gamma Power (Decay), W	1.02E+00	1.02E+00
Radioactivity, Ci	3.27E+02	3.28E+02
Alpha Activity, Ci	1.98E-04	1.98E-04
RCG, m^3 air	1.22E+11	1.21E+11
RCG, m^3 water	5.75E+08	5.75E+08
Chemical, m^3 water	1.26E+01	1.26E+01
(α, n) Neutron	1.45E-01	1.45E-01
S.F. Neutron	1.18E-01	1.18E-01

Conclusion and Future Work

- **MEDEAC**
  - Developed using Krylov Subspace Method to Replace ORIGEN code
  - Applied to UO_2 Fuel with Constant Flux of 1.0×10^{14}
  - Solution Comparison at 100 day with Fine Depletion and ORIGEN2
  - Library Converted from ORIGEN2 Library
  - MEDEAC Solution with 30 Day Depletion is Comparable with Fine Depletion Solution and ORIGEN2
  - It is concluded that MEDEAC can be used as an Alternative Code to ORIGEN2
- **Future Work**
  - Library Update
    - 1-G XS
    - RCG Data etc
  - Solver Update