KERMA calculation using TRIPOLI-4® and kinematics distributions of secondary particles.

DE LA RECHERCHE À L'INDUSTRIE

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Tripoli-4® Monte Carlo Transport Code

Particles : Neutron, Photon, Electron, Positron

Neutron : - GP Files up to 20 MeV (default upper energy)

Neutron Data Library treatment :

1/ NJOY2016 + CALENDF :

- **RRR reconstruction and Doppler : NJOY2016 (RECONR+BROADR)**
- **TSL Treatment NJOY2016/THERMR**
- **Probability Tables in URR provided by CALENDF**

2/ GALILÉE-1 (since 2021) :

- **Reconstruction, Doppler, PT (URR), TSL**

Photon : - Photo-Atomic reactions (EPDL97 library), no treatment

- Thick Target Bremsstrahlung

- Photonuclear reactions (semi-relativistic treatment) ENDF/B-VII library,
recent libraries will be added (JENDL-5, TENDL-21,…), no treatment

Electron, Positron : EEDL + EADL + Mott Scattering, no treatment

KERMA : Kinetic Energy Release in MAtter

TRIPOLI-4® keyword : DEPOSITED_ENERGY (E_D)

it can be applied for : NEUTRON, PHOTON, ELECTRON, POSITRON

Energy carried by heavy charged particles (proton, alpha, recoiled…) is deposited locally by using the energy balance equation (the energy of the charged particles does not need to be sampled)

Energy Balance : $E_{D,n} = E_{proj,n} + Q - \sum_i E_{i,n} - \sum_j E_{j,\gamma}$

$E_{D,n}$: Kerma Neutron
$E_{proj,n}$: Neutron incident energy
$E_{i,n}$: Neutron outgoing energy
$E_{j,\gamma}$: Photon outgoing energy

If Photon is not transported, energy carried by photon is deposited locally (the same for electron and positron)

◆ **Pure neutron simulation : DEPOSITED_ENERGY NEUTRON**

The energy carried by the photons emitted in nuclear reactions is assumed to be deposited locally : $E_{D,n} = E_{proj,n} + Q - \sum_i E_{i,n}$

◆ **Coupled neutron/photon simulation : adding DEPOSITED_ENERGY PHOTON**

DEPOSITED_ENERGY NEUTRON : $E_{D,n} = E_{proj,n} + Q - \sum_i E_{i,n} - \sum_j E_{j,\gamma}$

DEPOSITED_ENERGY PHOTON : $E_{D,\gamma} = E_{proj,\gamma} + Q - \sum_i E_{i,n} - \sum_j E_{j,\gamma}$

LRFlag is taken into account

Nuclear Data : Neutron Transport libraries

Kinematics of outgoing particles :

1/ Neutron projectile :

Neutron :
- Elastic scattering : Angular distribution (MF4)
- Inelastic scattering : Angular distribution (MF4) in CoM
  Double Differential data (MF6)
- Fission : Energetic distribution (MF5) and Angular distribution (MF4)
  Double Differential data (MF6)
- (n,2n), (n,3n) : MF5 +MF4
  MF6
- other reactions : Double differential data (MF6 / Kalbach-Mann)

neutron kinematics are well described

Photon :
- Discrete inelastic scattering :
  (MF12 or MF13) + MF14. Restriction : Energies are given in laboratory frame → No spread
  MF6 : Impossible to reconstruct properly the gamma cascade

- Other reactions : Average multiplicities and Average distributions

Nuclear Data : Photon Transport libraries

Kinematics of outgoing particles :

2/ Photon projectile :

- Photon : - Photo-atomic data : OK (+ EADL – Relaxation data)
  - Photonuclear data : incorrect threshold for various reactions
    Kinematics : classical or relativistic

- Neutron : - The near-exclusive use of MT5 (MF3 + MF6) does not allow the kinematics to be built correctly
  Exception : TENDL-21 considers MT50 reaction for all nuclei (only for 8 nuclei in the ENDF/B-VII photonuclear library)

Coupled neutron-photon calculations : KINEMATIC_LIMITS (TRIPOLI-4 score) computes the energy deposited by neutrons in coupled neutron-photon calculations without actually having to simulate photons, based on the laws of kinematics.

Gamma Production in libraries

	JEFF-3.3 (562 nuclei)	ENDF/B-VIII (556 nuclei)	JENDL-5 (795 nuclei)	JEFF-40T1 (562 nuclei)	TENDL-21 (630 nuclei)
(n,gamma) *	1	141	98	1	0
(n,fission) *	~ 9 / 70		~ 79 / 92	~ 20 / 70	~ 5 / 90
Inelastic *	24	5	4	39	43
Coupled n/γ *	31	9	477	42	46

(n,gamma) * : No gamma production for radiative capture. MT5 or MT3 ?

(n,fission) * : No gamma production for induced fission. MT5 or MT3 ?

Inelastic* : Gamma missing in MF12 for discrete inelastic scatterings. Ex : Pu239 / ENDF/B-VIII
MF12 : MT51 →MT68 ; MF3 : MT51 →MT90
Incoherence with the ENDF-6 Format : Impossible to reconstruct gamma cascade

Coupled n/γ * : TRIPOLI-4® calculation crashes. Transport n/ γ. Neutron Source 14 MeV

JEFF40T1 Library

Unit Base interpolation for secondary energy distributions is needed

- Negative angular distributions (MF4) : B10, Gd156 & Pu240 (MT2), Mn55 (MT71)

- Wrong or missing Q-Values in MF3 : Cd114, Cd116, Gd155, Gd156, Gd157, Gd158, Gd160, Sn113, Th233

  → Question : Use of an official file for masses : Nubase ?

- Discrepancies on masses : C12, Cd106, Cd113, Li6, Xe134

- Discrete inelastic scattering in MF6 : 46 nuclei

- Missing or underestimated gamma production at threshold for MT91

  Ex : Ag109 ; Q-value : 1.524 MeV ; Threshold (MT91) : 1.539 MeV
  Gamma Prod @1.53 MeV : 2 keV
  second energy point 1.8 MeV
  → Between 1.53 and 1.8 MeV the gamma production is underestimated

- For many nuclei, energy distributions are unchanged between 30 MeV and 200 MeV

- Wrong normalizations of energy distributions : Sn120, Cu67

JENDL5 Library

Unit Base interpolation for secondary energy distributions is very often used

- Negative angular distributions (MF4) : N14, O16, Sb126, Ra223, Ra224, Ra225

- MF6 is extensively used for discrete inelastic scattering (658 nuclei)
  → Impossible to reconstruct gamma cascade

- Law 7 is used for MF6 / MT5 f(E,μ,E') : Tripoli-4 transforms Law7 in Law 1 f(E,E', μ)

- C13 : Threshold MT54 > Sn but No BreakUp Flag

- Gamma Yield < 1 for discrete inelastic scattering. Ex : Cs133, Gd155, Gd157,..
  Gd157 : MF6 MT51 : Ein: 5.488350e+04 ; Gamma Yield < 1 : 7.463000e-02
  Gd157 : MF6 MT51 : Ein: 2.000000e+07 ; Gamma Yield < 1 : 7.463000e-02

TENDL21 Library

Unit Base interpolation for secondary energy distributions is needed

- Q-value differs from Nubase for 2 nuclei : Pu246 (MT45), Th232 (MT112)
- Anisotropy (MF4) : Threshold (MF4) should be lower or equal to Threshold (MF3)
- Anisotropy (MF4) : Cu63/MT2, Tabulated data (E > 30 MeV), normalization > 1
  Pb208/MT2, Tabulated data (E > 1 MeV), normalization > 1
- Energy Distribution (MF5) / Number of precursor families. U235 MF1 : 8 ; MF5 : 6
- MF6 Normalization ≠ 1 : Ag113 (MT104), Cu67 (MT105), In114 (MT105), Mo93 (MT106)
- F19 MF12 : Gamma production reaction by reaction up to 4.63 MeV.
  Use of MF13/MT3 above 4.63 MeV
- N14 : Overestimation of gamma production for (n,alpha) reaction and underestimation of gamma production for radiative capture
- U233 : underestimation of gamma production in radiative capture

Depletion calculation GP / Activation Files + DD File

Question : Gamma production in Zr Clad.
Case of Zr90 inelastic scattering to 2.319 MeV excited state (Metastable state 0.8s)

Is a prompt or a delayed gamma ? MT53 : discrete inelastic to 2.319 MeV excited state.

Depletion calculation to provide delayed gamma.

JENDL-5 : MF6/MT53 without gamma production and use of MF10/MT4
to product metastable state → gammaProduction through decay
of the metastable stata

JEFF-3.3 : MF12/MT53 : Prompt gamma.
In a depletion calculation , if you calculate the production of Zr90M using
Activation File and a neutron flux, the calculation generates gamma decay
of the metastable state → Double production of this decay

TENDL-21 : MF12/MT53 : prompt gamma + MF8-10/MT4 : metastable state production
→ Double production of this decay

Conclusion & Improvements

- Unit Base Lin-Lin interpolation is more physical than Lin-Lin.
  This is the forced interpolation in NJOY/MCNP
- MF12/MT51-90 : Best way to reconstruct gamma cascade for discrete inelastic scattering
- Effort on secondary particles energy distributions for Ein > 20-30 MeV
- Threshold and kinematics for photonuclear reactions
- The use of MT3 or MT5 induces complicated energy release calculations

Thank you for your attention